

Validation of CALPUFF in the Near-Field

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TABLE OF CONTENTS

1.	INTRODUCTION	1
2.	PURPOSE OF THE MODEL VALIDATION STUDY	2
3.	STUDY LOCATION	3
4.	STACK PARAMETERS AND EMISSIONS DATA	4
4.1	Source Description	4
4.2	Hourly Emissions, Stack Exit Velocities, and Stack Exit Temperatures	5
4.3	Magnitude of Stack Emissions	7
5.	SO ₂ MONITORING DATA	8
5.1	Description of Monitors	8
5.2	Use of Monitored SO ₂ Concentrations for Background and Model Validation	8
6.	METEOROLOGICAL DATA	10
6.1	Processing of Meteorological Data for AERMOD	11
6.2	Processing of Meteorological Data for CALPUFF	12
6.2.1	Initial Guess Wind Fields	12
6.2.2	Step1 Wind Fields	12
6.2.3	Step 2 Wind Fields	12
7.	AERMOD AND CALPUFF MODEL SETUP	14
7.1	AERMOD Model Setup	14
7.2	CALMET/CALPUFF Model Setup	14
7.2.1	Meteorological Modeling Domain	14
7.2.2	BIAS	15
7.2.3	TERRAD	15
7.2.4	R1, R2, RMAX1, RMAX2	16
8.	MODEL VALIDATION	17
8.1	Model Validation Statistics	18
8.1.1	Statistics Applied in Model Validation Parts 2 and 3	18
8.1.2	Statistics Applied in Model Validation Part 4	20
8.2	Model Validation Results Based on Actual Monitored Concentrations (Part 1)	21
8.3	Model Validation Results Based on EPA's AERMOD Validation Procedures (Part 2)	23
8.4	Model Validation Results Based on Protocol for Determining the Best Performing Model (Part 3)	24
8.4.1	Operational Component	24
8.4.2	Scientific Component	25
8.4.3	Composite Performance Measure (CPM)	27
8.5	BOOT Statistical Model Validation Results (Part 4)	27
9.	SUMMARY AND CONCLUSION	31
9.1	Comparison of Model Performance in Predicting the Upper-End Concentration Distribution	31
9.2	Evaluation of Under-Prediction Bias	32
9.3	Comparison of Model Performance with Large 1-Hour Concentration Data Sets ...	32

REFERENCES	34
FIGURES AND PHOTOS.....	36
APPENDIX A.....	52
Example AERMOD Modeling File	52
APPENDIX B.....	59
CALMET and CALPUFF Inputs.....	59
APPENDIX C	62
Determination of Robust High Concentrations (RHC).....	62

1. INTRODUCTION

This report describes a near-field validation study of the CALPUFF air dispersion model and evaluates its performance as compared to that of EPA's guideline model AERMOD. The study area encompasses portions of the Delaware River Valley in Warren County NJ and Northampton County PA. The model evaluation utilized the following data collected between May 1, 1992 through May 19, 1993: hourly sulfur dioxide (SO₂) measurements from eight ambient monitors, hourly SO₂ emissions data from four facilities in the area, and hourly meteorological measurements from two locations. The databases used in this study have also been used in several other model validation studies involving a number of different models (EPA, 2003; TRC, 1994; Perry, et. al., 2005; CERC, 2007).

2. PURPOSE OF THE MODEL VALIDATION STUDY

Appendix W to Part 51 of the Code of Federal Regulations (CFR), “Guidance on Air Quality Models,” provides guidance on the use of CALPUFF as an alternative model in the near field; in this instance, the region surrounding the Martins Creek and Portland power plants (EPA, 2005). Section 3.2.2(b) discusses the three separate conditions when an alternative model can be approved for use. Condition 2 of the rule states:

“if a statistical performance evaluation has been conducted using measured air quality data and the results of that evaluation indicate the alternative model performs better for the given application than a comparable model in Appendix A.”

Therefore, the purpose of this model validation study was to evaluate the performance of CALPUFF in this study area and determine if its use is appropriate and produces predictions of greater accuracy than the Appendix A model AERMOD. An additional objective of the validation study was to determine whether or not CALPUFF is biased towards underestimating measured SO₂ concentrations at this location¹.

¹ Appendix W to Part 51 CFR, Section 3.2.2e provides that an alternative refined model may be used if, among other requirements, “[a]ppropriate performance evaluations of the model have shown that the model is not biased toward underestimates;” subsection e does not technically apply as this subsection only applies to Condition 3, see Section 3.2.2b.

3. STUDY LOCATION

The study area is located approximately 80 km north of Philadelphia PA and 90 km west of New York City, NY near the town of Belvidere NJ. The Delaware River Valley transects the area with the higher terrain on either side of the river. The valley floor descends from 280 ft amsl level at the northern portion of the modeling grid to 220 ft amsl at the southern boundary. Along the study area's northern boundary is the Kittatinny Ridge with elevations up to 1550 ft above mean sea-level (amsl). The terrain on the west side of the Delaware River rises approximately 500 ft above the valley floor. The terrain to the east is generally higher than that to the west of the Delaware River. Significant terrain features on the east side of the Delaware River Valley near the Martins Creek Power Plant rise up to 1000 ft above the valley floor. Terrain features to the east of the Delaware River include Scotts Mountain (1281 ft amsl) and Jenny Jump Mountain (1070 ft amsl).

The model study area is shown in Figure 1. Figure 1 displays the terrain features and the locations of the four SO₂ emitting facilities included in the modeling, the meteorological stations, and the ambient SO₂ monitors. The Town of Belvidere, NJ is near the center of the map and a portion of Kittatinny Ridge is visible in the upper left corner.

Several aerial photos have been included in this report to provide a greater understanding of the region's terrain. Photo 1 shows a view of the Pennsylvania Martins Creek Power Plant looking to the east-southeast towards New Jersey with Scotts Mountain in the background. The area of Scotts Mountain is the location of seven of the eight SO₂ monitors. Photo 2 shows the Pennsylvania Portland Power Plant with New Jersey in the background. Photo 3 was taken looking south through the center of the study area. The Portland Power Plant is in the foreground and the Martins Creek Power Plant is in the background. The location of AMS-8 is on the elevated terrain along the right boarder of the photo. The last photo, Photo 4, is a view of Portland Power Plant through the Delaware Water Gap in Kittatinny Ridge. These photos clearly show there are significant terrain features in the study area. These terrain features generate the non-steady state wind fields that affect the transport and dispersion of plumes emitted from the Martins Creek and Portland Power Plants.

4. STACK PARAMETERS AND EMISSIONS DATA

4.1 Source Description

Hourly SO₂ emissions data for the model evaluation period were recorded at four facilities in the study area between May 1, 1992 and May 19, 1993. During the 1992-93 time period the Martins Creek Power Plant consisted of four units². Units 1 and 2 were each 1815 MMBtu/hr boilers that burned bituminous coal and vented to one 600 ft stack. During the validation study, Units 1 and 2 were limited by the Pennsylvania State Implementation Plan to emitting no more than 4.0 lbs of SO₂ per MMBtu. Units 3 and 4 were each 7721 MMBtu/hr oil-firing boilers that vent to separate 600 ft stacks. Units 3 and 4 were limited to no more than 1 percent sulfur oil (1.14 lbs of SO₂ per MMBtu). These three stacks were subject to aerodynamic building downwash due to the two hyperbolic, natural-draft cooling towers at the site. However, the curved shape of the cooling towers and their distance from the three stacks limited their downwash affects. The amount of downwash caused by the cooling towers was judged by EPA to be of such a small magnitude that the AERMOD performance evaluation studies using the Martins Creek data were classified as a non-downwash database (EPA, 2003; Perry, et. al., 2005).

The Portland Power Plant consisted of two bituminous coal-fired boilers, Unit 1 has a maximum heat input of 1659 MMBtu/hr and Unit 2 has a maximum heat input of 2511 MMBtu/hr. Each unit vents to its own 400 ft stack and was limited to emitting no more than 4.0 lbs per MMBtu of SO₂ during the validation study. Each stack is above their calculated GEP stack height and therefore not subject to building downwash.

The two smaller facilities included in the study were the Warren County Resource Recovery Facility (WCRRF) and the Hoffmann-LaRoche Facility. The WCRRF Facility consists of two municipal waste-firing 88 MMBtu/hr combustion units with an allowable emission rate of 19.8 lb/hr. The SO₂ emissions from the Hoffmann-LaRoche Facility during the validation study were from a 350 MMBtu/hr cogeneration unit with a maximum allowable SO₂ emission rate of 380 lbs/hr.

Table 1 summarizes the fixed stack parameters for the facilities.

² Units 1 and 2 at Martins Creek Power Plant were shutdown in September 2007.

Table 1. Source Characteristics

Source	UTM Coordinates (Zone 18, NAD-27)		Base Elev. (ft amsl)	Stack Height (m)	Stack Dia. (m)
	East (km)	North (km)			
Martins Creek Units 1 and 2	491.020	4,515.910	240	182.9 (600 ft)	5.30
Martins Creek Unit 3	491.123	4,516.030	240	182.9 (600 ft)	6.90
Martins Creek Unit 4	491.190	4,516.068	240	182.9 (600 ft)	6.90
Portland Unit 1	493.349	4,528.506	294	122.0 (400 ft)	2.84
Portland Unit 2	493.335	4,528.554	294	122.0 (400 ft)	3.79
Hoffmann LaRoche	494.050	4,521.040	340	59.4 (195 ft)	2.7
WCRRF Unit 1 and 2	498.950	4,518.500	570	76.2 (250 ft)	1.87

4.2 Hourly Emissions, Stack Exit Velocities, and Stack Exit Temperatures

Hourly SO₂ emission rates, exit velocities and stack temperatures were determined for each of the stacks at the four facilities. Generally, Continuous Emissions Monitors (CEMs) were used to obtain emissions data, sometimes in combination with hourly load data, and fuel sulfur content. The hourly SO₂ emission rates, stack temperatures, and exit velocities for all sources were obtained from EPA's website containing the 2003 AERMOD evaluation study (EPA, 2003) data:

<http://www.epa.gov/scram001/7thconf/aermod/martin.zip>.

Review of the CEM emissions data used in previous validation studies (TRC, 1994; EPA, 2003) discovered significant errors in the hourly SO₂ emission rate used for Portland Unit 1. Unit 1's hourly CEM data for each hour used in these studies was totaled for each month. The monthly SO₂ emission totals were compared to other emissions data provided by owners of the Portland Power Plant for the same May 1992 through May 1993 time period. One source of data was monthly coal use and coal sulfur content data contained in Reliant Energy's (now RRI Energy) May 3, 2001 response to a January 10, 2001 letter from EPA Region III (Reliant Energy, 2001). This information was requested by EPA pursuant to a CAA Section 114 investigation. Similar data, certified as accurate by the Vice-President of Metropolitan Edison Company, then owner of the Portland Power

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Plant, is contained in the 1992 and 1993 emissions data submitted by MetEd/GPU to the Pennsylvania Department of Environmental Resources (MetEd/GPU, 1993 and 1994). Major differences were found in the June 1992 through April 1993 monthly totals between these data sources and the SO₂ emissions used in the previous validation studies. These differences are given in Table 2.

Table 2. Comparison of Portland Unit 1's Monthly Actual SO₂ Emissions and the Monthly CEM Data Used in Previous Validation Studies

Year	Month	Coal Fired (tons)	% Sulfur of Coal	Reported Actual ^a (tons)	Previous Validation (tons)	Ratio of Actual to Validation Emissions
1992	May	2,468	2.01	89.5	85.8	1.04
1992	June	31,292	1.94	1095.8	637.0	1.72
1992	July	33,313	1.97	1184.6	511.0	2.32
1992	Aug.	25,264	1.9	866.4	447.8	1.94
1992	Sept.	20,984	2.23	844.6	372.7	2.27
1992	Oct.	27,946	2.17	1094.6	483.8	2.26
1992	Nov.	29,028	1.59	833.1	402.9	2.07
1992	Dec.	32,514	2.01	1179.6	576.0	2.05
1993	Jan.	22,564	1.95	794.2	404.6	1.96
1993	Feb.	30,081	1.87	1015.3	413.1	2.46
1993	March	32,427	1.91	1117.9	480.6	2.33
1993	April	30,755	1.8	999.2	474.6	2.11
1993	May	19,144	1.8	622.0	482.9	1.00 ^b
			Total =	11,736.9	5,772.8	

a. Actual SO₂ emissions calculated from Reliant's reported 1992-93 coal use and sulfur content of coal, and emission factor of 36.1 lb/ton.

b. Ratio of 1.00 assumed because no actual SO₂ emissions data for the specific period from May 1 thru May 19, 1993 is available.

The June 1992 through April 1993 data used in the previous validation studies had only 112 hours when the SO₂ emissions from Unit 1 were more than 50 percent of its allowable rate (1.6 percent of its hours in operation). This is far below the historical average and supports the conclusion that the SO₂ emissions data between June 1, 1992 and April 30, 1993 used in previous validation studies for Portland Unit 1 was flawed data.

As a result, the hourly CEM emissions data of Unit 1 was multiplied by the monthly ratio of actual to validation emissions value in the last column of Table 2. No inaccuracies were found with Portland Unit 2's hourly CEM SO₂ emissions data used in the previous validation studies.

4.3 Magnitude of Stack Emissions

A total of 52,101 tons of SO₂ was emitted from these four facilities during the validation period of May 1, 1992 to May 19, 1993. The largest one source of SO₂ emissions during the validation period was the single stack that vents Martins Creek Units 1 and 2 (a total of 20,270 tons). The next largest stack emissions were from Portland Unit 2 (12,939 tons) and Portland Unit 1 (11,737 tons).

While potentially major emitters of SO₂, Martins Creek Units 3 and 4 were relatively minor sources during the validation period. Unit 3 accounted for only 5.6 percent and Unit 4 accounted for only 6.6 percent of the total SO₂ emissions. Unit 3 was shutdown for 85.0 percent of the time and Unit 4 was shutdown 83.1 percent of the time during the validation study. Units 3 and 4 only operated at an 80 percent load or higher during approximately five percent of the validation study.

The Hoffmann-LaRoche Facility emitted only 837.1 tons of SO₂ during the validation study. Emissions of SO₂ from the WCRRF were negligible. The relative SO₂ emissions by facility during the validation study are summarized below:

- Martins Creek Power Plant Units 1 through 4 – 26,588 tons (51.0 percent of total)
- Portland Power Plant Units 1 and 2 - 24,675 tons (47.4 percent of total)
- Hoffmann-LaRoche – 837.1 tons (1.6 percent of total)
- WCRRF – 0.4 tons (~ 0.0 percent of total)

5. SO₂ MONITORING DATA

5.1 Description of Monitors

Ambient SO₂ measurements were collected from a network of eight monitoring stations. The locations of these monitors are shown in Figure 1.

The AMS-5, 7, 9, 10, 11, 12, and 13 monitors are all sited on Scotts Mountain, east to southeast of Martins Creek Power Plant and south of the Portland Power Plant. The elevations of these monitors range from 1,120 to 1,236 ft amsl. All monitors are well above the stack tops of the Martins Creek stacks (840 ft amsl) and the Portland Power Plant stacks (694 ft amsl). Therefore, these monitors represent a complex terrain plume/receptor relationship.

The AMS-8 monitor is located west of the Delaware River, 5.5 km to the northwest of Martins Creek Power Plant and 11 km southwest of Portland Power Plant. Its elevation of 810 ft amsl is much lower than the other monitors. AMS-8 is unique as compared to the other SO₂ monitors located on Scotts Mountain for the following reasons:

(1) The elevation of AMS-8 is near the stack-top elevation of the Martins Creek and Portland Power Plant stacks. Therefore, it is below the final height of the plumes emitted from these facilities and, unlike the other seven monitors, does not represent a complex terrain receptor.

(2) Emissions from the Portland Power Plant were principally responsible for elevated SO₂ concentrations measured at AMS-8. Examination of the meteorological conditions that occurred when AMS-8 measured its highest SO₂ concentrations during the validation period consistently showed winds blowing from the northeast quadrant, the direction of the Portland Power Plant. All of AMS-8's top 25 1-hour concentrations had concurrent SODAR and AMS-8 10 meter wind direction measurements out of the northeast quadrant.

5.2 Use of Monitored SO₂ Concentrations for Background and Model Validation

Background SO₂ concentrations were determined on an hourly basis from the monitoring network. The lowest hourly reported station(s) concentration was used as the hourly background concentration in order to reflect the regional-scale contributions from distant sources, rather than from the four facilities modeled. Each hour's designated hourly background concentration was subtracted from the observed hourly concentrations at all stations. The resulting 1-hour SO₂ concentration was used as the monitored values for the validation study.

Table 3 provides a summary of the locations and measured SO₂ concentration data obtained from the monitoring network during the period May 1, 1992 through May 19, 1993. The table shows that all monitors frequently contributed to the determination of the background value. Table 3 also shows there was a high level of data capture at the monitors.

Table 3. Locations and Data Summary of the SO₂ Monitors ^{NAD-27}

Monitor	UTM Coord. (km)		Elevation (ft amsl)	Hours of Data ^a	Data Capture	Hours Used for Background ^b
	East	North				
AMS-5	495.51	4,513.68	1,160	9,080	98.5%	1,547
AMS-7	493.90	4,513.20	1,236	9,038	98.1%	1,323
AMS-8	486.50	4,519.75	810	8,903	96.6%	3,152
AMS-9	492.70	4,513.44	1,215	8,995	97.6%	2,805
AMS-10	492.44	4,511.19	1,116	9,115	98.9%	2,557
AMS-11	495.40	4,515.18	1,170	9,090	98.6%	1,624
AMS-12	495.30	4,513.88	1,200	9,091	98.6%	2,675
AMS-13	496.43	4,514.50	1,120	9,093	98.7%	1,558

a. The total number of hours for the study was 9,216 hours (May 1, 1992 through May 19, 1993).

b. If two or more monitors had equal, low concentrations, then both stations were counted as measuring the background concentration.

A comparison of the long-term (May 1, 1992 – May 19, 1993) monitored to modeled concentrations is of limited usefulness. The long-term SO₂ concentrations measured at AMS-5 thru AMS-13 ranged from 20.8 ug/m³ to 24.8 ug/m³ before the background values were subtracted out, and from 9.1 ug/m³ to 13.1 ug/m³ after the background values were subtracted out. The detection level of the SO₂ monitors is approximately 16 ug/m³. In addition, the monitor's baseline (zero) can drift up to 26 ug/m³. These factors, in combination with the method used to estimate the hourly background values introduce a great deal of uncertainty in the monitor's long-term concentrations. This uncertainty is not a concern for shorter averaging times. The 1-, 3-, and 24-hour concentrations of interest are of a much higher magnitude than the annual average concentrations. Therefore, in this validation study the importance of the models reproducing long-term monitored concentrations is not as significant as reproducing the short-term averaging times (1, 3, and 24-hour).

6. METEOROLOGICAL DATA

Similar to previous validation studies at this site (TRC, 1994; EPA, 2003; Perry, et. al., 2005; CERC, 2007), meteorological data collected from May 1, 1992 through May 19, 1993 were used. The SODAR and 10 meter tower data from AMS-4 (see Figure 1) were both used in the meteorological preprocessor programs of the CALPUFF and AERMOD models. The AMS-4 site is located 2.5 km to the west-southwest of the Martins Creek Power Plant. AMS-4 is within the Delaware River valley at a base elevation of 320 feet. The SODAR data consists of wind speed and wind direction at 30 meter height increments from 90 meters to 420 meters above-ground. The 10 meter tower data consist of 10 meter wind speed, wind direction, standard deviation of the horizontal wind direction (sigma-theta) and temperature data.

To help capture the three-dimensional local and mesoscale wind fields, wind measurements taken at the AMS-8 meteorological tower were also input into CALMET. AMS-8 is located 6 km to the northwest of the Martins Creek facility and 10.6 km southwest of the Portland Power Plant (see Figure 1). It is on the valley ridge to the west of the Delaware River at a base elevation of 810 feet. At AMS-8, tower temperature, wind speed and wind direction were collected at the 10 meter level.

Concurrent twice daily upper air meteorological soundings from the Albany, NY, Sterling, VA, and Atlantic City, NJ National Weather Service (NWS) stations provided the remaining data needed for input into AERMET and CALMET.

Examining wind roses generated from this data can provide a better understanding of the complex wind flows within the modeling domain. Figure 2 contains a wind rose of the 10 meter AMS-4 data collected between May 1, 1992 and May 19, 1993. Not surprisingly, these low-level winds in the valley show a pronounced up-valley/down valley (northeast/southwest) flow. The SODAR data from the 150m level at AMS-4 is shown in Figure 3. The 150 meter SODAR level (840 ft amsl) is approximately equivalent in height above mean sea-level to the following: the height of the AMS-8 10 meter meteorological data, the height of the valley ridge running along the west of the Delaware River, and the top of the stacks that vent Units 1-4 at Martins Creek Power Plant. Winds at this level still show a strong terrain influence and the resulting up-valley/down valley winds.

The higher level 300m SODAR wind rose shown in Figure 4 displays more of a synoptic pattern with minimal valley influence. Winds at this level (1300 ft amsl) are above the highest peaks to the east of the Delaware River Valley. They are also representative of plume transport winds during some meteorological conditions. The final wind rose in Figure 5 summarizes the 10 meter wind speed and direction data from AMS-8 (810 ft amsl). While taken at the same height above ground as the AMS-4 10 meter data (Figure 2), these winds show little of the in-valley influence shown at AMS-4. The lower level winds at the AMS-8 ridge location more closely resemble the regional, synoptic wind direction distribution shown in Figure 4.

These four wind roses illustrate a wind field that varies dramatically in both the vertical and horizontal directions. Additional documentation of the existence of complex wind fields in the modeling study area can be found in the report *The Existence of Complex Wind Fields in the Region Surrounding the Portland Power Plant Site and the Use of CALPUFF Existence of a Complex Wind Field at the Portland Power Plant Site* (NJDEP, 2010).

6.1 Processing of Meteorological Data for AERMOD

The AERMET “profile” file from EPA’s 2003 AERMOD evaluation study (EPA, 2003) was used. This dataset containing the AMS-4 SODAR wind measurements between 90 m and 420 m is available at <http://www.epa.gov/scram001/7thconf/aermod/martin.zip>.

Similar to the 2003 and 2005 AERMOD validations studies, the AMS-4 10 meter tower was used as the primary surface station for generating the “surface” meteorological file for input into AERMOD with the AMS-8 10 meter level as first backup and NWS data as the final backup. However, the “surface” meteorological data file was reprocessed with the most recent version of the AERMET meteorological processing system to reflect changes in guidance on generating the data and updates to AERMET since the 2003 EPA study (TRC, 2008).

AERSURFACE (version 08009) was used to determine the surface characteristics (surface roughness, albedo and Bowen ration) for the area surrounding the AMS-4 meteorological tower. Using the 1992 USGS National Land Cover Data Sets (NLCD92) data, surface roughness for the site was determined in 30 degree sectors for a 1 km radius circle around the observing site. The earlier 2003 EPA study had used a 3 km radius circle and only two sectors. The Bowen ratio and albedo were determined based on the average characteristics over a 10 by 10 km square centered on the observing site as opposed to a 3 km radius circle used in the earlier 2003 EPA study. The Bowen ratio was determined on a monthly basis and the meteorological year was characterized as wet or dry based on a thirty year period of climatological data for Allentown.

The meteorological data were processed with the AERMET meteorological preprocessor (version 06341) to provide the “surface” meteorological data file for input into AERMOD. The surface file consists of hourly wind speed, wind direction and temperature data, surface characteristics (albedo, surface roughness length and Bowen ratio) and the derived boundary layer parameters (heat flux, Monin-Obukhov length, friction velocity, convective velocity scale, convective and mechanically-driven boundary layer heights and vertical potential temperature gradient above the boundary layer).

6.2 Processing of Meteorological Data for CALPUFF

The CALMET model was used to develop the parameters for the three-dimensional meteorological grid. The meteorological grid includes meteorological parameters, surface parameters, and terrain elevations for each hour. This three-dimensional meteorological grid was calculated by CALMET in three steps, as discussed in the following subsections.

6.2.1 Initial Guess Wind Fields

The SODAR data from AMS-4 was incorporated into CALMET using the subroutine PROF2UP. PROF2UP constructs a CALMET ready UP.DAT vertical wind and temperature file. The three additional upper air data sites (Albany, NY, Atlantic City, NJ and Sterling, VA) were also used for developing the initial guess wind fields of the three-dimensional meteorological grid.

6.2.2 Step1 Wind Fields

The geophysical data, as processed by the TERREL, CTGPROC and MAKEGEO pre-processors were used to account for the effects of terrain and surface characteristics. TERREL reads raw terrain data, calculates the elevation of the center of each grid cell in the modeling domain, and writes a processed data file. The elevation of the center of the grid cells were calculated using sixteen 7.5 minute (24,000:1) DEM terrain data files with a horizontal spacing of 10 meters. CTGPROC reads land use data, calculates weighted land use for each grid cell in the modeling domain, and writes a processed data file. USGS National Land Cover Datasets (NLCD 92) which have a 30 meter resolution were used to calculate the weighted land use for each grid cell.

MAKEGEO reads the processed data files from CTGPROC and TERREL. MAKEGEO calculates weighted surface characteristics and writes those data as well as the terrain elevations to a processed data file, MAKEGEO.DAT. The MAKEGEO.DAT file is used by the CALMET model to modify the initial guess wind fields in developing the step 1 wind fields. A value of 2.7 kilometers was selected for TERRAD, the radius of influence of terrain features. This value approximates the distance from the valley floor to the top of the valley that is used in modifying the initial guess wind fields to develop the step 1 wind fields of the three-dimensional meteorological grid.

6.2.3 Step 2 Wind Fields

Meteorological observations (surface data, and upper air data) are used to modify the step 1 wind fields to develop the step 2 wind fields of the three-dimensional meteorological grid. Besides the 10 meter data from AMS-4 and AMS-8, surface meteorological data from the NWS stations at Allentown/Lehigh Valley PA, Newark NJ, and Wilkes-Barre,

DEP

PA were input into CALMET. The combination of on-site SODAR data and surface meteorological stations, NWS Upper Air data and surface stations, fine-grid terrain data, and fine-grid land use data resulted in an appropriate representation of the three-dimensional flow in the modeling domain.

7. AERMOD AND CALPUFF MODEL SETUP

7.1 AERMOD Model Setup

The AERMOD input file from EPA's 2003 AERMOD evaluation study (EPA, 2003) was input into the EPA approved version 07026 of AERMOD. An example AERMOD output file from this validation study is in Appendix A.

7.2 CALMET/CALPUFF Model Setup

Modeling was performed with the latest EPA approved version of the CALPUFF modeling suite; CALMET/CALPUFF Version 5.8, Level 07063 and CALPOST Version 5.6394, Level 070622. CALMET version 5.8 was used to develop the wind fields for the model validation. Table B.1 in Appendix B lists the options selected when making the CALMET run. Predictions at the eight monitoring locations were done with CALPUFF version 5.8. Table B.2 in Appendix B lists important options selected when making the CALPUFF runs in this study.

7.2.1 Meteorological Modeling Domain

The 37.8 km by 40 km CALMET/CALPUFF modeling domain is shown in Figures 6 and 7. The values used in CALMET to define the horizontal and vertical grid resolution within this modeling domain are listed in Table B.1. The selected values provide enough detail to adequately capture the horizontal and vertical gradients of the complex winds at this location. The modeling grid used a horizontal resolution of 200 meters. There were a total of 12 vertical layers. The vertical resolution in the lower levels of the atmosphere was defined with grid cells between 0 – 20m, 20 – 40m, 40 – 80m, 80 – 135m, 135 – 195m, 195 – 255m, 255 – 315m, 315 – 405m, 405 – 1000m, 1000 – 1500m, 1500 – 2200m, and 2200 – 3000m. This level of detail allowed CALPUFF to incorporate the multi-level SODAR measurements at AMS-4. Table 4 lists the coordinates of the meteorological grid.

Table 4. CALMET Meteorological Domain

DATUM	WGS-84
Southwest Corner	
XORIGKM	UTM 473.700 km Zone 18
YORIGKM	UTM 4508.700 km Zone 18
Number of Grid Cells	
NX	189
NY	200
Horizontal Grid Spacing	
	0.200 km
Vertical Grid Spacing ^a	
1	20 m
2	40 m
3	80 m
4	135 m
5	195 m
6	255 m
7	315 m
8	405 m
9	1,000 m
10	1,500 m
11	2,200 m
12	3,000 m

a. Top of each cell

7.2.2 BIAS

The layer-dependent bias factor (BIAS) settings for each vertical cell determines the relative weight assigned to the vertically extrapolated surface meteorological observations and upper air soundings. The initial guess field is computed with an inverse distance weighting of the surface and upper air data. The bias affects the vertical interpolation of surface and upper air observations. The biases selected were -1 for the first layer, 0 for the next two layers, and +1 for the remaining 9 layers. Use of a -1 bias eliminates the influence of the upper air measurements in the ground to 20 meter layer of the CALMET grid. Use of a +1 bias for the highest 9 layers (80m to 3000m) eliminates the influence of the surface air measurements in the 80 m to 3000 m layers. A bias of 0 means there will be no bias in applying the surface and upper air measurements to the 20 m to 80 m layers.

7.2.3 TERRAD

TERRAD is defined as the radius of influence of terrain features. TERRAD is the distance used in computing the kinematic effects (IKINE), the slope flow effects

DEP

(ISLOPE), and the blocking effects (IFRADJ) on the wind field. TERRAD should be set to the approximate distance from the valley floor to the top of the valley. In general, TERRAD is going to be of the order of 5 to 12 grid cell lengths expressed in kilometers. If TERRAD is smaller than this, the grid cell size should be reduced.

The valley near the Martins Creek Generating Station has hills to the east that are about 2.8 kilometers from the valley floor and hills to the west that are about 3.0 kilometers. The valley near the Portland Generating Station has hills to the east that are about 1.0 kilometers from the valley floor and hills to the west that are about 2.0 kilometers. A value of 2.7 kilometers was selected for TERRAD to account for the terrain variations.

7.2.4 R1, R2, RMAX1, RMAX2

CALMET uses an inverse-distance squared method to determine the influence of observations in modifying the step 1 wind field. R1 and R2 are the distances from observation stations at which the observations and the step 1 winds are equally weighted. R1 controls the weighting of the surface layer and R2 controls the weighting of the upper layers.

RMAX1, and RMAX2 determine the radius of influence over land in the surface layer, and over land in layers aloft. Therefore, an observation is excluded if the distance from the observation site to a given grid point exceeds the maximum radius of influence.

Because the terrain is rugged near the sources, relatively small values were appropriate for the weighting factors for near-field transport. The maximum distances and relative weightings of observations (i.e., R1, R2, RMAX1, and RMAX2) are presented in Table 5.

Table 5. CALMET Weighting Factors

PARAMETER	DESCRIPTION	VALUE (KM)
Terrad	Radius of Influence of Terrain Features	2.70
RMAX1	Maximum Radius of Influence Over Land (Surface)	2.00
RMAX2	Maximum Radius of Influence Over Land (Aloft)	2.00
R1	Relative Weighting (Surface)	1.00
R2	Relative Weighting (Aloft)	1.00

In CALPUFF, the atmospheric chemistry option that would convert SO₂ to sulfate was turned off. Also, there was no wet or dry deposition calculated. The option that produces “ISCST3-like” plume dispersion with the Pasquill-Gifford dispersion coefficients was not used. Instead, the option that utilized similarity theory based dispersion coefficients (MISP=2) and probability density function convective boundary layer conditions

(MPDF=1) were selected. Selection of these options results in CALPUFF using a plume dispersion methodology similar to AERMOD.

8. MODEL VALIDATION

The Guideline on Air Quality Models (EPA, 2005), Section 3.2.2(d) references two principal documents for guidance on determining the acceptability of an alternative model such as CALPUFF for an individual case. One of the references is the document *ASTM D 6589: A Standard Guide for Statistical Evaluation of Atmospheric Dispersion Model Performance* (EPA, 2000). The techniques described in this document are more appropriate for evaluating a model with tracer test data, not a long-term, continuous concentration data set with a limited number of monitors such as the Martins Creek data base. The other document referenced in Section 3.2.2(d) is *Protocol for Determining the Best Performing Model* (EPA, 1992). This document, which is also referenced in Section 3.2.1(a) of the Guideline on Air Quality Models, recommends the use of various statistical techniques in evaluating a model's performance when predicting peak concentrations at individual monitoring locations. The statistical measures from this document have been included in the model validation.

Additional measures of model accuracy have also been used in this model validation that reflect historical techniques or techniques recently used by EPA in the AERMOD model validation studies. Emphasis was placed on statistics that demonstrate the model's ability to reproduce the upper end of the concentration distribution. These concentrations are most important in regulatory applications and the determination of whether short-term National Ambient Air Standards (NAAQS) are violated. The model validation consists of four parts:

Part 1: CALPUFF and AERMOD predicted impacts compared to actual monitored concentrations with no statistics applied.

Part 2: CALPUFF and AERMOD predicted impacts compared to monitored concentrations applying the statistical methodology used in the two principal AERMOD validation studies (EPA, 2003) (Perry, et. al., 2005).

Part 3: CALPUFF and AERMOD predicted impacts compared to monitored concentrations following guidance in EPA document *Protocol for Determining the Best Performing Model* (EPA, 1992).

Part 4: CALPUFF and AERMOD predicted 1-hour impacts compared to monitored concentrations using statistical performance metrics calculated by the computer program: BOOT Statistical Model Evaluation Software Package, Version 2.0 by Chang and Hanna (2005).

The ability of CALPUFF and AERMOD to predict SO₂ concentrations was judged on their combined performance in each of these four components (i.e., weight-of-evidence).

8.1 Model Validation Statistics

8.1.1 Statistics Applied in Model Validation Parts 2 and 3

The robust high concentration (RHC) is designed to represent a “smoothed” estimate of the highest concentration based on an exponential fit to the upper end of the concentration distribution. The RHC attempts to represent a stable estimate of the highest concentration, one that mitigates the unwanted influence of unusual events. As stated in the AERMOD validation study (Perry, et. al., 2005), “for regulatory applications, a good model would produce a concentration distribution parallel to the slope of the measured distribution and produce high-end concentrations (RHCs) that are similar to that of the observations.”

The RHC for modeling validation purposes was first defined in the paper *A Statistical Procedure for Determining the Best Performing Air Quality Simulation Model* (Cox and Tikvart, 1990). The RHC is computed as follows:

$$\text{RHC} = X(N) + [X - X(N)] [\text{Ln}((3N-1)/2)]$$

where:

$X(N)$ = Nth highest value

X = average of the N-1 highest values

N = number of values exceeding a threshold value

Previous validation studies that have used the RHC have selected a value of $N=26$ as the best representation of the upper-end distribution of concentrations (USEPA, 2003) (Perry, et.al., 2005). While N in these previous studies has been set equal to 26, the selected value must adequately define the slope of the upper end of the distribution of concentrations. The Cox and Tikvart paper, as well as the USEPA guidance document *Protocol for Determining the Best Performing Model* (USEPA, 1992) suggest that when there are greater than 25 values above a designated threshold value, the value of N could be 26. However, both state that the selection of N being equal 26 is arbitrary. In order to provide an accurate estimate of the RHC, William Cox (personal communication), an author of the above paper, recommended that the slope of the tail distribution of all 1-hour, 3-hour and 24-hour monitored concentrations be evaluated on an individual basis. This evaluation is contained in Appendix C of the document.

The calculation of an annual average RHC has limited usefulness in this study. The uncertainties in establishing the annual average for modeling purposes include: the detection level of the SO_2 monitors, the method hourly background values are estimated, and the limited number of data points (eight monitors). Therefore, no annual RHC was used. Instead, each model's maximum annual average impact was compared to the measured maximum annual average monitored concentration at the eight monitors.

To assist in the model comparison, the fractional bias for each model and averaging time was also calculated. The fractional bias (FB) is a dimensionless number that will range from -2 (extreme over-prediction) to 2 (extreme under-prediction). It is a fundamental measure of the discrepancy between the monitored and model predicted concentrations and is defined as:

$$FB = 2[(\text{observed} - \text{predicted})/(\text{observed} + \text{predicted})]$$

A FB of -0.67 is equivalent to an over-prediction by a factor of 2, a FB of 0.67 is equivalent to an under-prediction by a factor of 2. A FB of 0.0 represents a perfect prediction. The absolute fractional bias (AFB) represents the absolute value of the FB. The AFB does not account for the over or under-predictions of the model, just the absolute discrepancy between monitored and modeled concentrations. The EPA 1992 protocol document recommends using the RHC values to calculate a model's FB.

The composite performance measure (CPM) is discussed in the USEPA guidance document *Protocol for Determining the Best Performing Model* (USEPA, 1992). It is divided into two components, an operational component and a scientific component. The operational component compares the highest measured RHC at any monitor with the highest model predicted RHC at any monitor. This is done for both the 3-hour and 24-hour averaging times. The scientific component only examines the 1-hour average concentrations that occur at the monitors under different meteorological conditions.

The operational component is considered the more important of the two and is given twice the weight of the scientific component.

$$CPM = 1/3 [\text{avg. of scientific AFB}]_{1\text{-hour}} + 2/3 [(\text{network wide AFB})_{3\text{-hour}} + (\text{network wide AFB})_{24\text{-hour}}]$$

The *Protocol for Determining the Best Performing Model* (USEPA, 1992) document goes on to recommend that a bootstrap procedure be used to estimate the uncertainty in the CPM for each model. The problem with the use of the bootstrap technique occurs when the RHC is used in the CPM. The document requires use of the RHC in both the operational and scientific components of the CPM. The bootstrap technique involves re-sampling the monitoring and model prediction data and creating hundreds of artificial "trial" years. Model statistics are then generated for each of these trial years. With this data, standard error for each of the model performance statistics is calculated.

However, as discussed earlier, in this study the arbitrary selection of N=26 to define the RHC was not done. The range of monitored concentrations was visually evaluated for each averaging time on an individual basis and a value of N selected that best defined the slope of the upper-tail distribution of concentrations. Therefore, to be consistent, each of the "trial" year's tail distribution of concentrations would need to be evaluated on an individual basis and a value of N selected for the calculation of the RHC.

Because there is no computer program available to evaluate the slope of the tail concentrations and select the correct value of N, each trial year's range of concentrations

DEP

would need to be examined visually and a determination of N made. Such an effort is clearly impractical (William Cox, personal communication). In this study the confidence that one model's predictions are superior to another will be based on the results of the variety of statistical measures described earlier, a weight of evidence argument.

Network wide Q-Q plots were also generated. Network wide Q-Q plots are created by ranking concentrations predicted at all eight monitors by each model with the observed concentrations at all eight monitors by rank. Because ranked modeled and monitored concentrations are paired regardless of when and where they occur, the comparison is independent of time and space. A 1:1 slope in the Q-Q plot represents good model performance. Special emphasis is placed on matching the monitored values in the upper end of the concentration distribution. Q-Q plots were generated for the 1-, 3-, and 24-hour averaging times.

8.1.2 Statistics Applied in Model Validation Part 4

The fourth part of the model validation study used the BOOT Statistical Model Evaluation Software Package, Version 2.0 (Chang, Hanna, 2005) as distributed with the Model Validation Kit (Oleson, 2005). The original BOOT software program was based on recommendations by Hanna (1989), but has been upgraded to include additional performance measures, and the implementation of the ASTM (2000) model evaluation procedure.

The BOOT software package calculates a variety of performance measures. In this analysis the following statistics generated by the BOOT program were evaluated: the fraction of predictions within a factor of two of observations (FAC-2), the normalized mean square error (NMSE), fractional bias (FB), the under-predicting component of the fractional bias (FB_{FN}), and the over-predicting component of the fractional bias (FB_{FP}).

The FAC-2 gives the fraction of predictions that are within a factor of two of observations (FAC-2). The ability of a model to predict at least 50 percent of the concentrations within a factor of two of the observed concentrations is a fundamental requirement of model acceptability (EPA, 1992). The lower the NMSE, the better the model's overall ability to make accurate predictions. A NMSE value of 0.0 indicates no scatter between observed and predicted concentrations (i.e., a perfect model). A NMSE less than 1.0 implies the magnitude of the scatter is less than the mean concentration. FB_{FP} and FB_{FN} are always positive and, when combined, are equivalent the FB. While the FB is a measure of mean relative bias or systematic bias, the NMSE is a measure of both mean relative bias and random scatter. FB_{FP} and FB_{FN} are always positive and when combined are equivalent the FB.

Bootstrap resampling was used to estimate the confidence limits of a performance measure. The boot-strapping algorithm was run to generate the 95% confidence limits for each models FB. The 95 percent confidence level was used to test two hypotheses:

- when compared to observations, is the model's FB significantly different from zero,
- when compared, are the differences in FBs between the two models significantly different from zero (i.e., are the models predictions significantly different from each other?)

The last statistical performance measure evaluated was the correlation coefficient, a measure of the linear relationship between the observed and modeled concentrations. The correlation coefficient is most meaningful for the time-series data pairing. A correlation coefficient of one represents a perfect correlation between monitored and modeled values.

The program also includes an implementation of the ASTM statistical model evaluation procedure; however, due to the long term and limited number of monitors this was not used. These other statistical measures are more useful for tracer tests using monitors in series of arcs at downwind distances from the source.

8.2 Model Validation Results Based on Actual Monitored Concentrations (Part 1)

The first step in this portion of the model validation was the comparison of the network wide maximum and second-high monitored values with each model's actual maximum and second-high network wide predictions. The results of these comparisons are shown in Table 6. Except for the second high 24-hour, AERMOD under-predicts the high and second-high 3-hour and 24-hour concentrations. CALPUFF accurately predicts the high and second high 3-hour and high 24-hour concentrations, and over-predicts the second-high 3-hour impact. While both models under-predict the high and second-high 1-hour concentrations, CALPUFF does so by a smaller magnitude. Both models under-predict the annual monitored concentrations.

The composite ratio of CALPUFF of high and second-high predictions for all four averaging times is 1.01, with a range of 0.77 to 1.38. The composite ratio of AERMOD for the same four averaging times is 0.85, with a range of 0.70 to 1.00. These composite ratios, as well as the individual ratios, indicate CALPUFF more accurately predicts the highest measured concentrations and that AERMOD has a greater tendency to under-predict actual measurements than CALPUFF.

Table 6. Network Wide Ratio of CALPUFF and AERMOD High and 2nd High Modeled Concentrations to Observed High and 2nd High Concentrations

Averaging Time	Observed (ug/m ³)	CALPUFF		AERMOD	
		Model (ug/m ³)	Ratio	Model (ug/m ³)	Ratio
High 1-Hour	1823.5	1402.8	0.77	1271.8	0.70
2 nd High 1-Hour	1362.4	1240.2	0.91	1160.2	0.85
High 3-Hour	710.0	724.6	1.02	563.4	0.79
2 nd High 3-Hour	629.7	649.2	1.03	524.6	0.83
High 24-Hour	185.3	200.9	1.08	165.9	0.90
2 nd High 24-Hour	131.2	182.6	1.38	131.2	1.00
High Annual	13.1	11.31	0.86	11.15	0.85

The next step of this validation component was a comparison of all measured 1-hour observations greater than the monitor's detection level with model predictions as a function of atmospheric stability. Three sets of atmospheric stability were examined: unstable, neutral, and stable. The classification of atmospheric stability was based on the Monin-Obukhov length (L) data contained in the "surface" meteorological file that was input into AERMOD. This data used for the determination of L was from the AMS-4 surface meteorological station. Assuming an average surface roughness of 0.1 meters, the relationship of L to atmospheric stability was as follows: values of L between 0 and -65 were assumed unstable (Pasquill-Gifford [PG] stability class A, B, and C), values of L less than -65 and greater 65 were assumed neutral (PG stability class D), and values of L between 0 and 65 were assumed stable (PG stability class E and F) (EPA, 2007).

Of 9,216 validation hours (May 1, 1992 to May 19, 1993), 2,583 were classified as unstable, 2,239 hours classified as neutral, and 4,393 classified as stable. After removal of values at or less than the monitor's threshold of 16 ug/m³, 1,450 hours were classified as unstable, 1,046 hours classified as neutral, and 2,180 hours classified as stable. All modeled concentrations less than 16 ug/m³ were also set equal to 16 ug/m³. Data pairs with both observation (background subtracted) and predictions at the detection limit of 16 ug/m³ were ignored since by definition there is no difference for that pair.

Residual box plots represent a method of directly comparing modeled and monitored data. They are generated by calculating the ratio of each model's ranked maximum prediction at any of the eight monitors for an hour to the ranked maximum measured 1-hour concentration at any of the eight monitors.

Residual box plots showing the CALPUFF and AERMOD distribution of these ratios as a function of stability are shown in Figure 9. The significant points for each box plot indicate the 2nd, 16th, 50th, 84th, and 98th percentiles and the mean of the cumulative distribution of ratios. Figure 9 illustrated a generally better performance by CALPUFF than AERMOD. CALPUFF's unstable or neutral residual box plots both cross the "1" line, while AERMOD's residual box plots show every hour is under-predicted during

unstable and neutral conditions. During stable conditions CALPUFF under-predicts and AERMOD over-predicts.

8.3 Model Validation Results Based on EPA's AERMOD Validation Procedures (Part 2)

EPA conducted a number of validation studies when it was investigating the replacement of the ISC3 model as its primary guideline model with AERMOD. These AERMOD validation studies are described in the EPA report *AERMOD: Latest Features and Evaluation Results* (EPA, 2003) and the paper *AERMOD: A dispersion model for industrial source applications. Part II: Model performance against 17 field study databases* (Perry, et. al., 2005). The focus of these validations was the need for the model to predict the peak of the concentration distribution, unpaired in time and space. When using long-term continuous monitored data, such as the Martins Creek data set, EPA judged the performance of the models using two statistical measures, the network wide RHC, and the network wide quantile-quantile (Q-Q) plots.

Based on the factors discussed in Appendix C, N in the RHC equation has been set equal to 8 for calculating the network wide 3-hour RHC and set equal to 26 for calculating the network wide 24-hour RHC concentrations. Table 7 lists the ratio of AERMOD and CALPUFF's RHC predictions for 3-hour and 24-hour time periods to the RHC monitored values for the same time periods. To assist in the comparison, the FB for each model and averaging time is also provided in Table 7.

Table 7 shows that both models made fairly accurate predictions of the maximum RHC on a network wide basis. However, CALPUFF's predictions are demonstrated to be clearly superior to AERMOD for two reasons:

(1) CALPUFF's FBs and AFBs are lower for both the 3 and 24-hour averaging times and therefore, as discussed in Section 8.1.1, reflect a more accurate prediction of measured RHCs. The average of CALPUFF's FB is -0.035, AERMOD's is 0.155. The average AFB of CALPUFF's is 0.055, AERMOD's is 0.155.

(2) CALPUFF's RHC predictions are either at or modestly above the monitored RHC values. As in the Part 1 of the validation, AERMOD under-predicts both the 3 and 24-hour concentrations.

Table 7. Ratio of CALPUFF and AERMOD RHC to Network Wide Observed RHC^a

Averaging Time	CALPUFF			AERMOD		
	Model (ug/m ³)	Ratio to Obs.	FB	Model (ug/m ³)	Ratio to Obs.	FB
3-Hour	720.2	1.09	-0.09	570.0	0.86	0.14
24-Hour	183.7	0.98	0.02	158.1	0.84	0.17

a. Monitored RHCs: 3-hour = 659 ug/m³, 24-hour = 187.0 ug/m³.

The 1-hour, 3-hour, and 24-hour observations, and model predictions at each monitor location were ranked to generate the quantile-quantile (Q-Q) plots shown in Figure 8. In the figures the solid line indicates a one-to-one correspondence in the modeled and observed concentrations. The dashed lines on either side of the solid line indicate a factor of two overestimate by the model (upper line) and a factor of two underestimate by the model (lower line).

The Figure 8 shows that the predicted 1-hour and 3-hour concentrations are well within a factor of 2 of the monitored concentrations for both models. An under-prediction of monitored values occurs at lower concentrations for all three averaging times. There is a greater than factor of 2 under-prediction at the low concentration of the 24-hour values. The detection limit of the SO₂ monitors discussed earlier is responsible for a large part of the under-prediction by the models of the very lowest monitored 24-hour concentrations. Figure 8 shows that both models over-predict by less than a factor of 2 in the mid to upper range of measured 1-hour concentrations.

For the most part, the distributions of the predictions of AERMOD and CALPUFF are similar for all three averaging periods. The model predictions do deviate from each other at the upper range of concentrations. Concentrations predicted by CALPUFF tend to be higher than the AERMOD predictions, but only in the extreme upper range of observed concentrations.

8.4 Model Validation Results Based on Protocol for Determining the Best Performing Model (Part 3)

The *Protocol for Determining the Best Performing Model* is cited in the Guideline on Air Quality Modeling (EPA, 2005) as a document that provides statistical techniques for evaluating model performance for predicting peak monitored concentrations. Composite performance measures (CPMs) were calculated for the two models following the guidance contained in this document. The CPM has an operational and scientific component.

8.4.1 Operational Component

For the operational component, 3-hour and 24-hour RHCs concentrations were calculated for each of the eight monitors. When calculated at each monitor, AMS#12 had the highest RHC for 3-hour concentrations and AMS#8 had the highest RHC for 24-hour concentrations. As discussed in Appendix C, a RHC based on the 11 highest 3-hour concentrations (N=11) best represents the high end distribution of measured concentrations. At AMS#8, a RHC based on the 16 highest 24-hour concentrations best represents the high end distribution of measured concentrations.

The comparison between monitored and modeled RHC is given in Table 8. Both models over-predict the monitored 3-hour RHC and under-predict the monitored 24-hour RHC.

The location of CALPUFF's predicted maximum 3-hour RHC was able to match the location of the measured maximum 3-hour RHC (monitor AMS#12). The average absolute fractional bias in this operational component comparison, 0.245 for AERMOD and 0.21 for CALPUFF, indicates a slightly better performance by CALPUFF.

Table 8. Individual Monitor's Maximum Modeled RHC Compared to the Observed RHC ^a

Averaging Time	CALPUFF			AERMOD		
	Model (ug/m ³)	Ratio to Obs.	FB	Model (ug/m ³)	Ratio to Obs.	FB
3-Hour	658.3 (AMS#12)	1.30	-0.26	616.6 (AMS#7)	1.22	-0.21
24-Hour	165.5 (AMS#9)	0.85	0.16	147.4 (AMS#9)	0.76	0.28

a. Individual monitor's highest RHCs: 3-hour = 505.6 ug/m³ (AMS # 12), 24-hour = 194.6 ug/m³ (AMS#8)

8.4.2 Scientific Component

The scientific portion of the CPM examined the 1-hour RHC for monitors located in two types of terrain under three different atmospheric stabilities. The first set of monitors was located on terrain at or above the plume height of emissions from the principal sources of interest, the Martins Creek and Portland Power Plants. These monitors, AMS-5, -7, -9, -10, -11, -12, and -13, represent a complex terrain plume/receptor relationship. As shown in Table 3, the elevation of these monitors range from 1120 ft to 1236 ft amsl. The second set represents monitors located on terrain at the approximate stack top of the Martins Creek stacks (840 ft amsl) and the Portland Power Plant stacks (694 ft amsl). Only AMS-8 (810 ft amsl) met that requirement.

The tail distribution of monitored concentrations was examined and 1-hour RHCs determined for the complex terrain and stack top monitors for each of the three atmospheric stabilities derived using the technique described in Section 8.2 of the report. Appendix C contains graphs of the tail-end distributions and justification for the selected 1-hour RHCs.

Each models' 1-hour RHC predictions are compared to the complex terrain monitors RHC in Table 9. AERMOD severely under-predicts the 1-hour RHC during unstable conditions, the stability during which the highest 1-hour RHC occurred at the monitors. AERMOD over-predicts the monitors' RHC during neutral and stable conditions. CALPUFF accurately predicts the 1-hour RHC during unstable conditions and modestly over-predicts during stable conditions. CALPUFF over-predicts the 1-hour RHC during neutral conditions, but it should be noted that the lowest RHCs at these monitors occur during neutral atmospheric stability.

Table 9. 1-Hour Maximum Modeled RHCs Compared Observed RHC for the Complex Terrain Monitors ^a

Atmospheric Stability	CALPUFF			AERMOD		
	Model (ug/m ³)	Ratio	FB	Model (ug/m ³)	Ratio	FB
Unstable	1308.3	1.02	-0.02	428.2	0.33	1.00
Neutral	849.3	2.75	-0.93	439.5	1.42	-0.35
Stable	1177.1	1.23	-0.21	1247.4	1.31	-0.27

a. Complex terrain monitor's unstable 1-hour RHC = 1286.5 ug/m³, neutral 1-hour RHC = 309 ug/m³, stable 1-hour RHC = 955 ug/m³

The AERMOD and CALPUFF 1-hour RHC predictions are compared to the stack top monitor's 1-hour RHC in Table 10. AERMOD moderately to severely under-predicts the 1-hour RHCs at this monitor. AERMOD's under-prediction is highest during neutral conditions, the stability during which the highest 1-hour RHC occurred at AMS-8. As with the complex terrain monitors, CALPUFF does an excellent job of predicting the 1-hour RHC during unstable conditions. CALPUFF does under-predict the 1-hour RHC during neutral and stable conditions. However, the magnitude of its under-prediction during neutral conditions is much lower than AERMOD. The lack of meteorological data collected near the Portland Power Plant contributed to the models' inaccuracies in predicting maximum concentrations at the stack top monitor (AMS-8). As was discussed, emissions from Portland Power Plant have a major impact on concentrations measured at AMS-8.

Table 10. 1-Hour Maximum Modeled RHC Compared to Observed RHC for the Stack Top Monitor ^a

Atmospheric Stability	CALPUFF			AERMOD		
	Model (ug/m ³)	Ratio	FB	Model (ug/m ³)	Ratio	FB
Unstable	395.3	1.08	-0.07	237.8	0.65	0.43
Neutral	364.8	0.58	0.53	200.0	0.32	1.03
Stable	303.0	0.62	0.47	325.2	0.66	0.41

a. Stack top terrain monitor's unstable 1-hour RHC = 367.7 ug/m³, neutral 1-hour RHC = 627.2 ug/m³, stable 1-hour RHC = 490.6 ug/m³

Based on the results presented in Tables 9 and 10, the scientific component average absolute fractional bias for CALPUFF is 0.372. The scientific component average absolute fractional bias for AERMOD is 0.582.

8.4.3 Composite Performance Measure (CPM)

When both operational and scientific components are combined, the CPM for CALPUFF is the following:

$$\text{CPM} = 1/3 [0.372]_{1\text{-hour}} + 2/3 [(0.26)_{3\text{-hour}} + (0.16)_{24\text{-hour}}] = 0.405$$

AERMOD's CPM is calculated below.

$$\text{CPM} = 1/3 [0.582]_{1\text{-hour}} + 2/3 [(0.21)_{3\text{-hour}} + (0.28)_{24\text{-hour}}] = 0.521$$

The lower CPM of CALPUFF signifies that it is the superior performing model in predicting the impacts of SO₂ emissions from the Martins Creek and Portland Power Plants at the study area.

8.5 BOOT Statistical Model Validation Results (Part 4)

The fourth part of the model validation study involved the use of the BOOT Statistical Model Evaluation Software Package, Version 2.0 (Chang, Hanna, 2005). Several large datasets were evaluated with the BOOT software. The first was a time series comparison between the maximum measured 1-hour concentrations at any of the eight monitors (background subtracted) with the maximum model prediction at any of the eight monitors for the same hour. The highest monitored and modeled value for a given hour was considered the best test of model performance. Any hours with 1-hour concentrations of 16 ug/m³ or less after background was subtracted out were set equal to 16 ug/m³, the monitors' detection limit.

This dataset of 9216 hours was then modified by ranking the monitored and modeled concentrations and calculating the statistics on these pairings of values. In addition to a 16 ug/m³ detection threshold, an additional source of monitoring uncertainty is baseline (zero) drifts up to a magnitude of 26 ug/m³ (EPA, 2003). Therefore, to remove the influence of the low-end, uncertain monitoring values on the calculated statistics, only ranked monitored concentrations 42 ug/m³ and higher were included in the data set. A total of 2,449 hours remained. These hours were then divided into atmospheric stability categories using the Monin-Obukhov length (L) data from AMS-4 as discussed in Section 8.2. These ranked datasets consisted of 810 hours classified as unstable, 630 hours classified as neutral, and 1008 classified as stable.

Table 11 shows that for the hourly time series data pairing, both model's predictions are within a factor of two of observations (FAC-2) 68 percent of the time. The FB indicate both models over-predict, but CALPUFF's over-prediction is by a lower magnitude. The values of FB_{FP} and FB_{FN} indicate that under-prediction and over-prediction of observations contribute approximately equal amounts to the overall FB. The higher correlation coefficient of CALPUFF suggests it does a slightly better job of following the changes in each hour's maximum observed 1-hour concentration over time.

Table 12 summarizes the results for the ranked modeled and monitored concentrations comparison with all monitored concentrations less than 42 ug/m³ removed. As expected, the average of all 1-hour observations and predictions are significantly higher than the time series dataset. The average 1-hour concentration predicted by CALPUFF is closer to the observed average than AERMOD. The FAC-2s of both models are above 90 percent. The two models' NMSE are nearly identical. AERMOD's higher value of FB and FB_{FP} indicates a higher tendency to over-predict the entire set of 1-hour observations than CALPUFF.

Tables 13 through 15 summarize the results for the three atmospheric stability regimes. The average of the observed 1-hour concentrations for each of the three stabilities are fairly uniform, ranging from 94.4 ug/m³ (stable) to 104.7 ug/m³ (neutral). The average 1-hour concentrations predicted by CALPUFF for these three averaging times (88.8 ug/m³ to 141.9 ug/m³) vary less than the range of AERMOD predictions (69.3 ug/m³ to 192.4 ug/m³). The FAC-2s of both models are extremely high for the unstable and neutral conditions, near or at 100 percent. For the stable condition, both models FAC-2 falls to the mid-50 percent range. The CALPUFF NMSEs for all three stabilities are lower than those of AERMOD, especially during stable conditions.

The unstable and neutral atmospheric stabilities, FB and FB_{FN} of AERMOD show significant under-prediction. An FB_{FP} of zero indicates that AERMOD under-predicted every hour during unstable and neutral conditions. AERMOD FB and FB_{FN} during stable conditions show a pronounced over-prediction of observed concentrations. This is not unexpected given AERMOD's large over-prediction of the average 1-hour observed concentrations during stable conditions. The over-prediction FB_{FP} component of the FB far exceeds the under-prediction component FB_{FN}.

CALPUFF's 1-hour average predictions and FBs for each of the three stabilities listed in Tables 13 through 15 reflect more accurate model predictions and superior model performance than AERMOD. The FB values indicate CALPUFF has a tendency to over-predict during unstable hours, but makes relatively accurate predictions during both neutral and stable conditions. The values of FB_{FP} and FB_{FN} demonstrate a more even distribution between under and over-prediction of 1-hour concentrations by CALPUFF as compared to AERMOD, whose predictions for a given stability are dominated by either under-prediction (unstable and neutral) or over-prediction (stable).

Table 11. Summary of Performance Measures for the Network 1-Hour Time Series

	Observed	CALPUFF	AERMOD
Average	40.80	41.71	44.32
Highest	1823.5	1402.8	1271.8
2 nd Highest	1362.4	1240.2	1160.2
FAC-2	n/a	0.68	0.68
Correlation Coef.	n/a	0.128	0.103
FB	n/a	-0.022	-0.083
FB _{FN}	n/a	0.428	0.339
FB _{FP}	n/a	0.450	0.481

Table 12. Summary of Performance Measures for the Network 1-Hour Ranked

	Observed	CALPUFF	AERMOD
Average	99.5	112.7	121.3
Highest	1823.5	1402.8	1271.8
2 nd Highest	1362.4	1240.2	1160.2
FAC-2	n/a	0.91	1.00
NMSE	n/a	0.30	0.29
FB	n/a	-0.125	-0.198
FB _{FN}	n/a	0.097	0.042
FB _{FP}	n/a	0.221	0.240

Table 13. Summary of Performance Measures for the Network 1-Hour Ranked - Unstable

	Observed	CALPUFF	AERMOD
Average	101.8	141.9	72.7
Highest	1823.5	1402.8	475.1
2 nd Highest	717.9	1086.3	387.9
FAC-2	n/a	1.00	0.998
NMSE	n/a	0.45	0.52
FB	n/a	-0.329	0.333
FB _{FN}	n/a	0.021	0.333
FB _{FP}	n/a	0.350	0.000

Table 14. Summary of Performance Measures for the Network 1-Hour Ranked –Neutral

	Observed	CALPUFF	AERMOD
Average	104.7	110.4	69.3
Highest	820.10	765.60	495.20
2 nd Highest	471.60	742.40	428.10
FAC-2	n/a	1.00	1.00
NMSE	n/a	0.14	0.24
FB	n/a	-0.053	0.407
FB _{FN}	n/a	0.085	0.407
FB _{FP}	n/a	0.138	0.00

**Table 15. Summary of Performance Measures for the
Network 1-Hour Ranked - Stable**

	Observed	CALPUFF	AERMOD
Average	94.4	88.8	192.4
Highest	1362.4	1240.2	1271.8
2 nd Highest	741.5	1199.6	1160.2
FAC-2	n/a	0.565	0.576
NMSE	n/a	0.33	1.07
FB	n/a	0.061	-0.683
FB _{FN}	n/a	0.236	0.001
FB _{FP}	n/a	0.175	0.684

The confidence limits of the FBs in Tables 11 through 15 were calculated using the bootstrap resampling technique. As discussed earlier, the boot-strapping algorithm was run to generate the 95% confidence limits (2.5th and 97.5th percentiles) to test whether, when compared to observations, each model's FB significantly differs from zero and, when compared to each other, are the differences in FBs between the two models significantly different from zero.

Figure 10 graphically depicts the FB confidence limits for the two datasets; the network 1-hour time series and the network 1-hour ranked. The BOOT Statistical Model output indicated that for the network 1-hour ranked, both CALPUFF and AERMOD's FBs are significantly different than zero, CALPUFF and AERMOD's FBs are significantly different from each other. Because CALPUFF's FB is closer to zero, it would be considered the better performing model. The model output also shows that the two models' network 1-hour time series FBs are not significantly different from each other. However, the CALPUFF FB is not significantly different from zero, while the AERMOD FB is significantly different from zero.

Figure 11 graphically depicts the FB confidence limits for the three datasets; the network 1-hour ranked unstable conditions, the network 1-hour ranked neutral conditions, and the network 1-hour ranked stable conditions. The BOOT Statistical Model output indicated the only model with a FB not significantly different from zero is the CALPUFF neutral case. The CALPUFF stable case approaches very near but does not reach the zero line. The remaining cases, CALPUFF unstable atmospheric stability and all three stabilities for AERMOD, have FBs significantly different from zero. For all three stabilities the CALPUFF FBs are closer to zero than AERMOD indicating more accurate predictions and are significantly different than AERMOD's FBs.

Overall, Figures 10 and 11 and the BOOT model output indicate that there is a statistically significant difference in performance of the two models, and that CALPUFF is the better performing model.

9. SUMMARY AND CONCLUSION

This model validation establishes that use of CALPUFF for this application is appropriate, produces predictions of greater accuracy than AERMOD, and is not biased towards underestimating measured sulfur dioxide concentrations. In combination, the results summarized below clearly demonstrate CALPUFF's superior performance in this model validation in accordance with the requirements of Section 3.2.2(b) of Appendix W to Part 51 of the CFR. In addition, CALPUFF has been shown to have no overall bias towards under-prediction. Therefore, the use of CALPUFF as an alternative model in this study area and for these sources is appropriate.

9.1 Comparison of Model Performance in Predicting the Upper-End Concentration Distribution

Emphasis was placed on statistics that demonstrate the model's ability to reproduce the upper end of the concentration distribution because of their importance in regulatory applications and determining compliance with the NAAQS. The quantitative measures of the two models' accuracy in predicting the upper end distribution of monitored concentration in the first three parts of the validation study are summarized below:

Part 1 - Each model's average of the high and second-high ratio using actual monitored concentrations:

CALPUFF Ratios: 1-hour = 0.84, 3-hour = 1.03, 24-hour = 1.23, annual = 0.86;
AERMOD Ratios: 1-hour = 0.77, 3-hour = 0.81, 24-hour = 0.95, annual = 0.85.

Part 2 - Each model's FBs and modeled to monitored ratio using network wide RHC concentrations per EPA's AERMOD validation studies methodology:

CALPUFF FB: 3-hour = -0.09, 24-hour = 0.02,
Ratio: 3-hour = 1.09, 24-hour = 0.98.

AERMOD FB: 3-hour = 0.14, 24-hour = 0.17,
Ratio: 3-hour = 0.86, 24-hour = 0.84.

Part 3 - Each model's CPM as defined in the Guidance in the *Protocol for Determining the Best Performing Model*:

CALPUFF CPM = 0.405; AERMOD CPM = 0.521.

An FB or CPM closer to 0.00 denotes more accurate model predictions. In each instance, the FB or CPM is lower for CALPUFF indicating it is the better performing model.

Other results in Part 3 of the model validation indicate a greater skill by CALPUFF in predicting the location of maximum impacts. Table 8 shows the location of CALPUFF's predicted maximum 3-hour RHC matched the location of measured maximum 3-hour RHC (monitor AMS#12). CALPUFF also generally does better when predicting 1-hour concentrations at the stack top monitor (AMS-8) and the seven complex terrain monitors on Scotts Mountain during the three atmospheric stabilities.

9.2 Evaluation of Under-Prediction Bias

Examination of the ratio between the model's predicted and monitored actual concentration or RHC gives an indication of whether the model is prone to under or over-prediction. A ratio greater than 1 signifies over-prediction by the model, a ratio less than one indicates under-prediction. The average ratios from Tables 6 through 10 of the first three parts of the model validation are summarized below:

Part 1 - Each model's composite of modeled to monitored ratios for all averaging times:
CALPUFF = 1.01; AERMOD = 0.875.

Part 2 - Each model's ratio using network wide RHC concentrations per EPA's AERMOD validation studies methodology:
CALPUFF: 3-hour = 1.05, 24-hour = 0.98;
AERMOD: 3-hour = 0.82, 24-hour = 0.84.

Part 3 - Each model's average operational and scientific ratio RHCs as defined in the Guidance in the *Protocol for Determining the Best Performing Model*:
CALPUFF: operational = 1.15, scientific = 1.24;
AERMOD: operational = 0.995, scientific = 0.79.

These ratios demonstrate that AERMOD is much more inclined to under-predict maximum concentrations than CALPUFF, and that CALPUFF's predictions of maximum impacts are relatively unbiased.

9.3 Comparison of Model Performance with Large 1-Hour Concentration Data Sets

In Part 4 of the model validation, the superior model performance of CALPUFF was also evident. The BOOT Statistical Model Evaluation Software Package was used to generate statistics for five large 1-hour data sets. The average 1-hour concentration predicted by CALPUFF for each of the datasets is closer to the average monitored value than the average AERMOD prediction except for the unstable case. The FAC-2s of both models were relatively high for four of the five datasets. Both models had a lower FAC-2 for the stable case. The NMSE indicated less scatter in the CALPUFF predictions for all three atmospheric stabilities.

For all five data sets, CALPUFF's FBs were closer to zero than AERMOD's. When evaluated by stability class, AERMOD's bias towards under-predicting during unstable and neutral conditions is significant and generally consistent with the findings in Part 1 and 3 of this model evaluation. AERMOD also showed an extreme tendency to over-predict 1-hour concentrations during stable conditions. While CALPUFF tended to over-predict during unstable conditions, its accuracy in predicting 1-hour concentrations during neutral and stable conditions was excellent, as reflected by the low FBs.

Evaluation of the 95 percent confidence level of each model's FB found that in four of the five datasets examined, CALPUFF's accuracy in predicting monitored concentrations was significantly better than that of AERMOD. The FB 95 percent confidence levels also indicated that in two of the five datasets examined, CALPUFF's FB was not significantly different from zero. Conversely, in all five cases AERMOD's FB was significantly different than zero.

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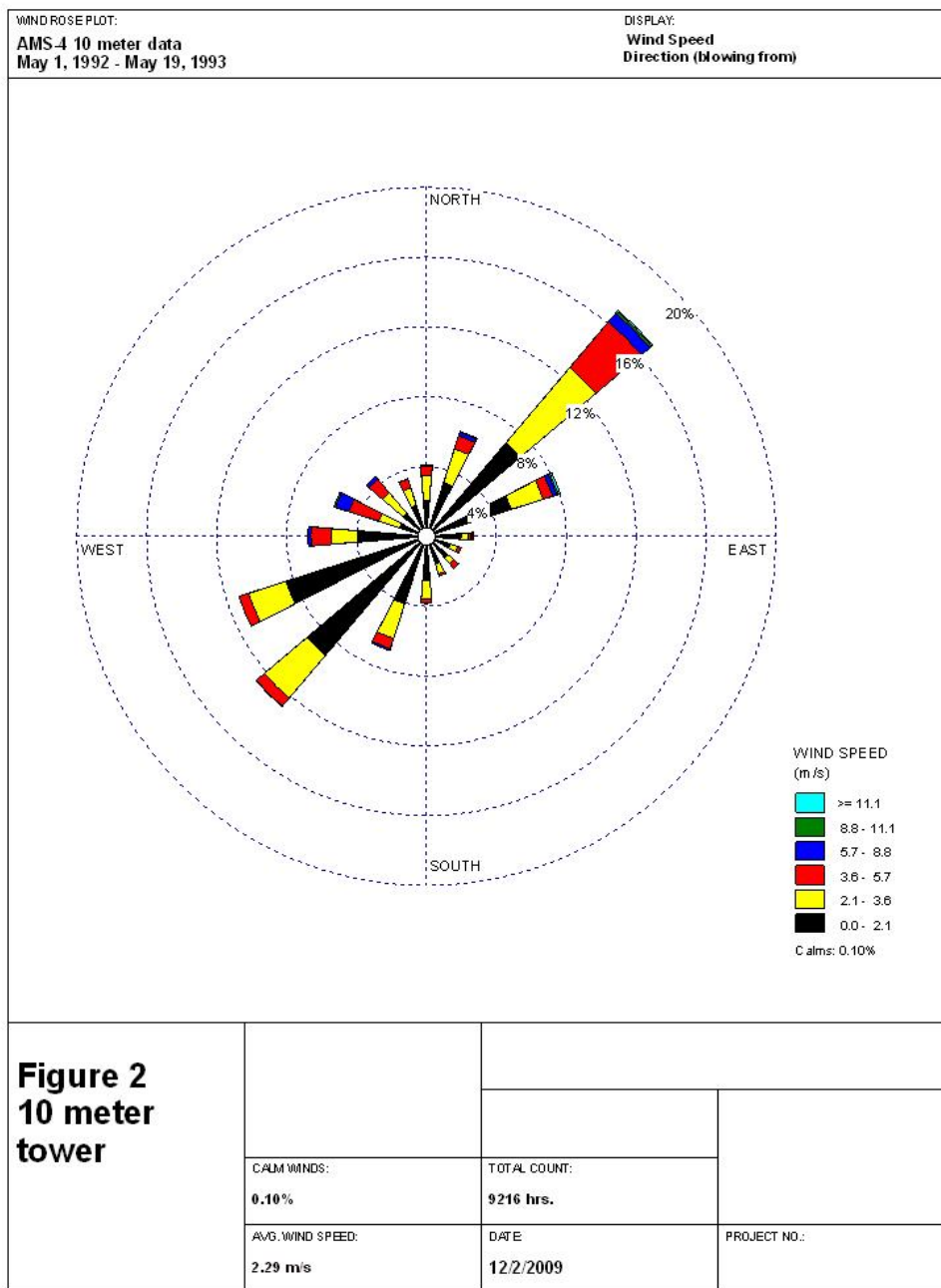
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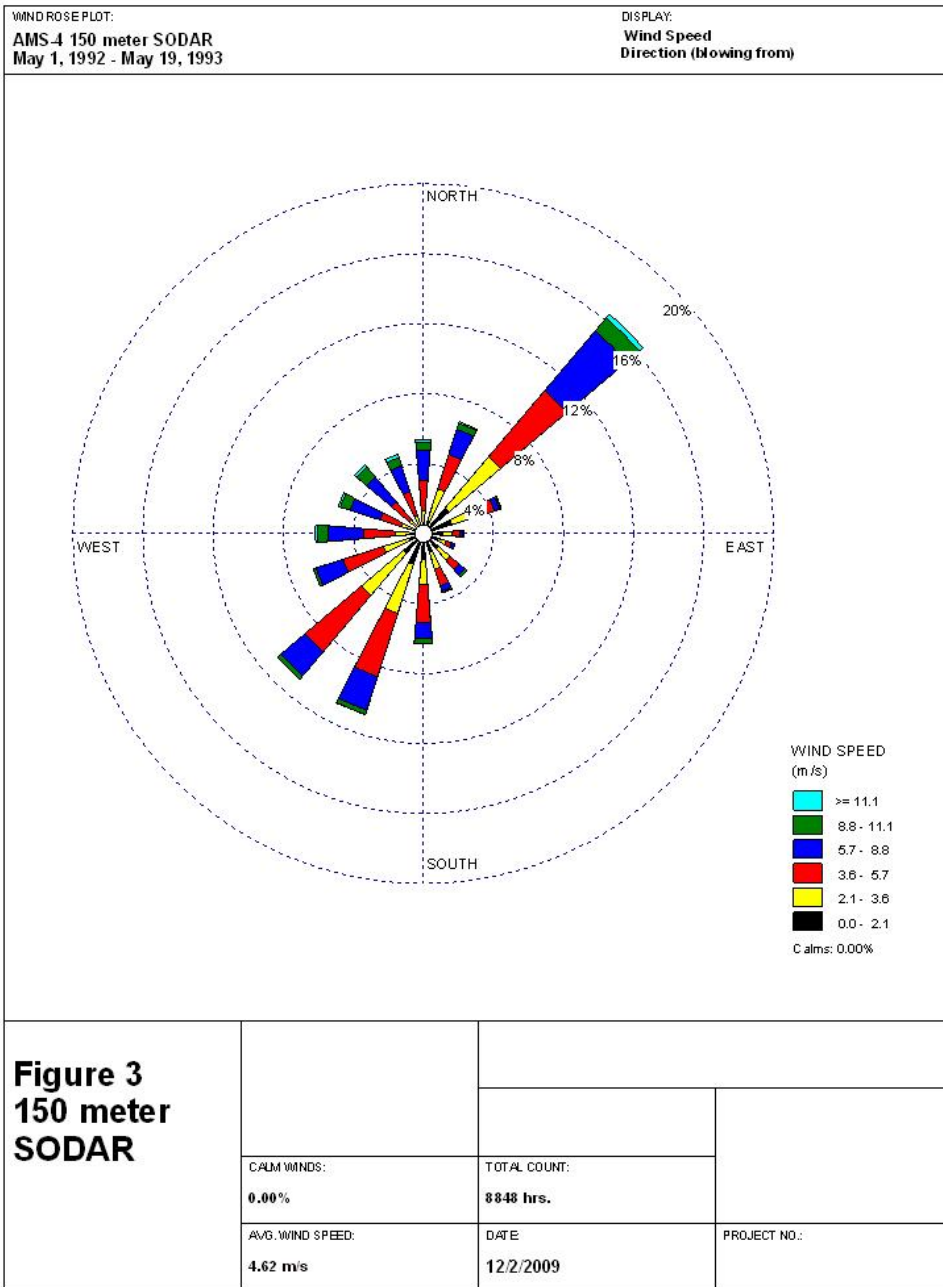
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FIGURES AND PHOTOS

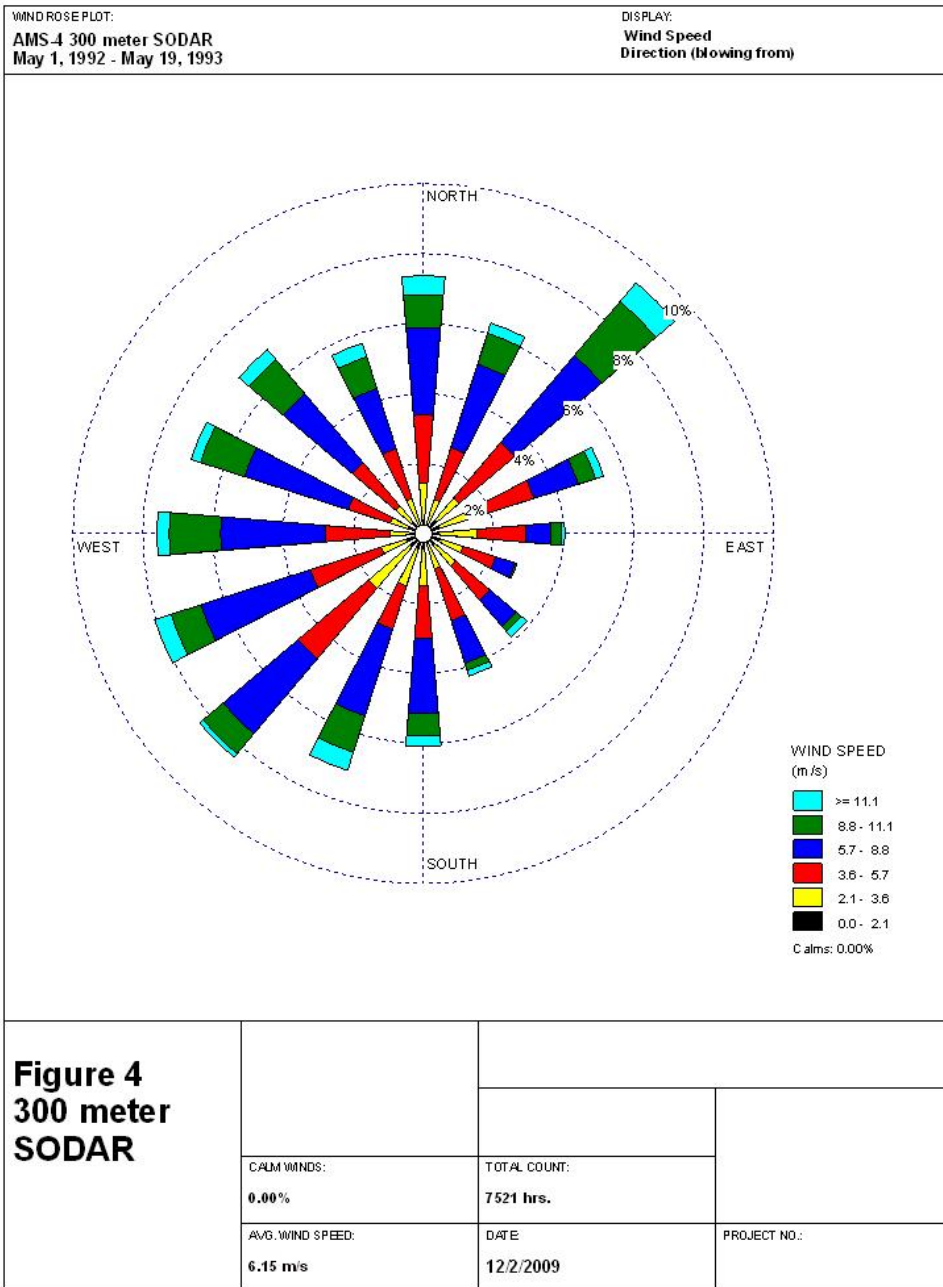


Figure 1. Location of Sulfur Dioxide Sources, Monitors, and Meteorological Stations Used in the Model Validation Study

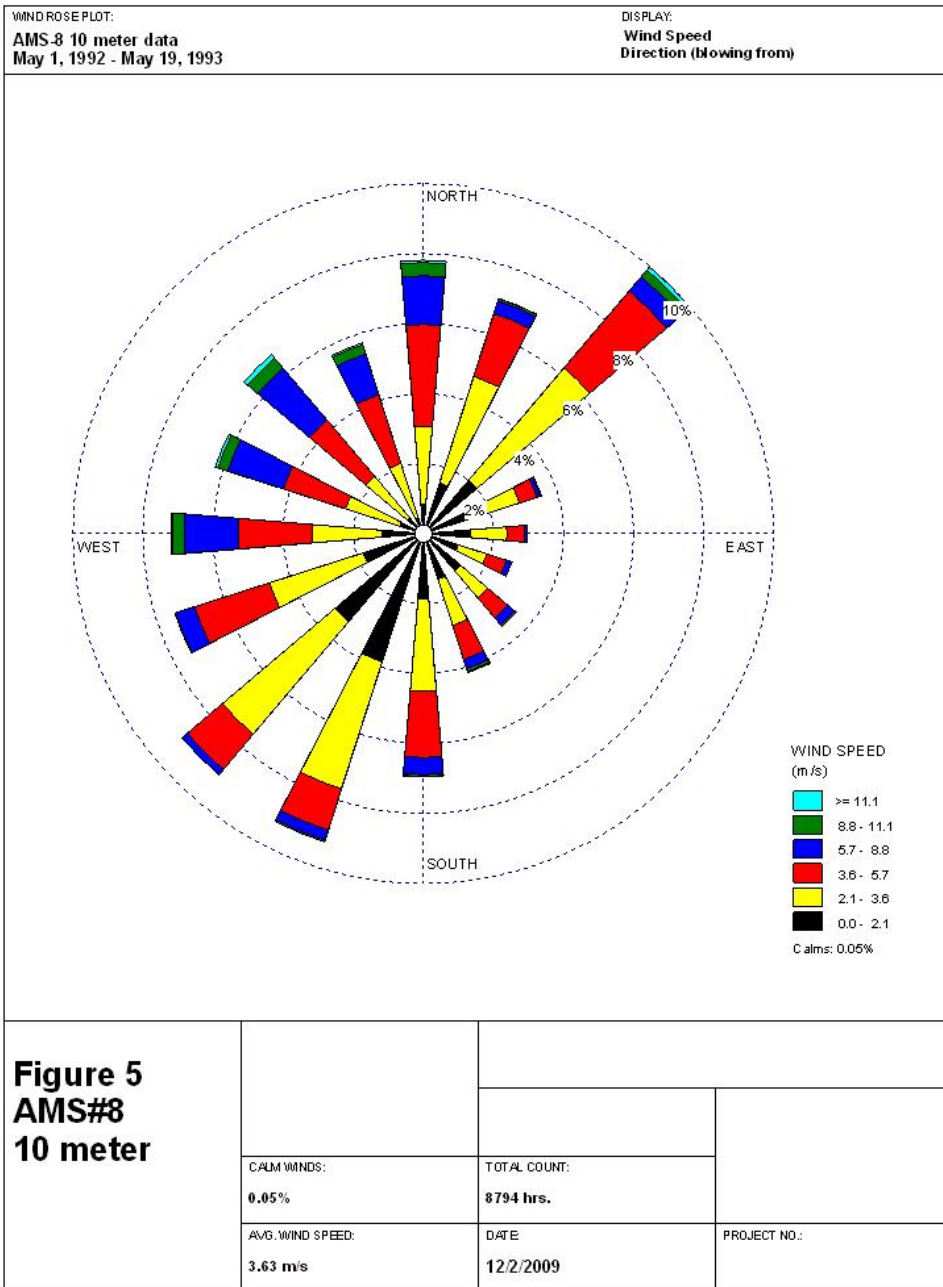




WRPLOT View - Lakes Environmental Software



WRPLOT View - Lakes Environmental Software



WRPLOT View - Lakes Environmental Software

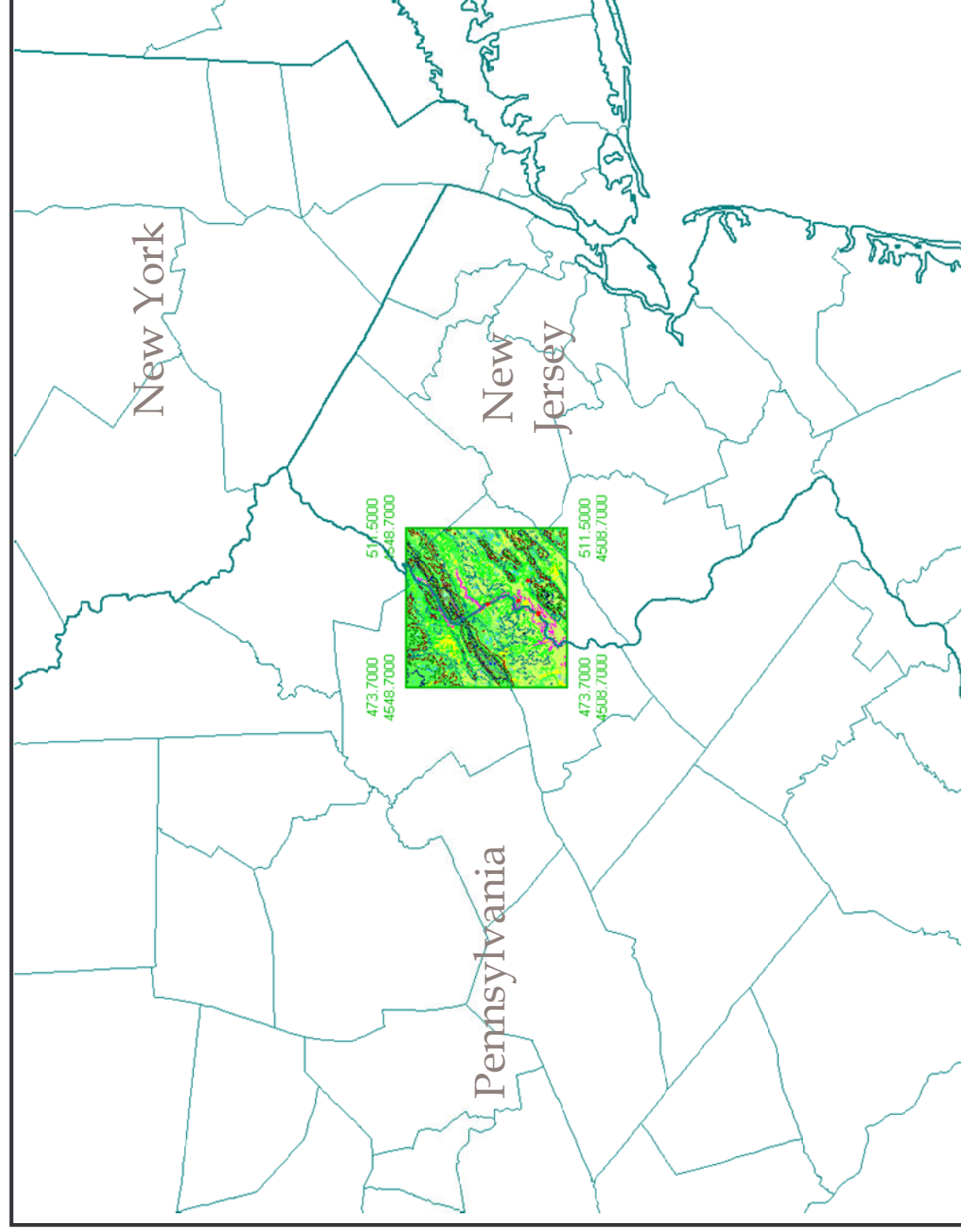


Figure 6. Location of CALMET/CALPUFF Meteorological Modeling Domain

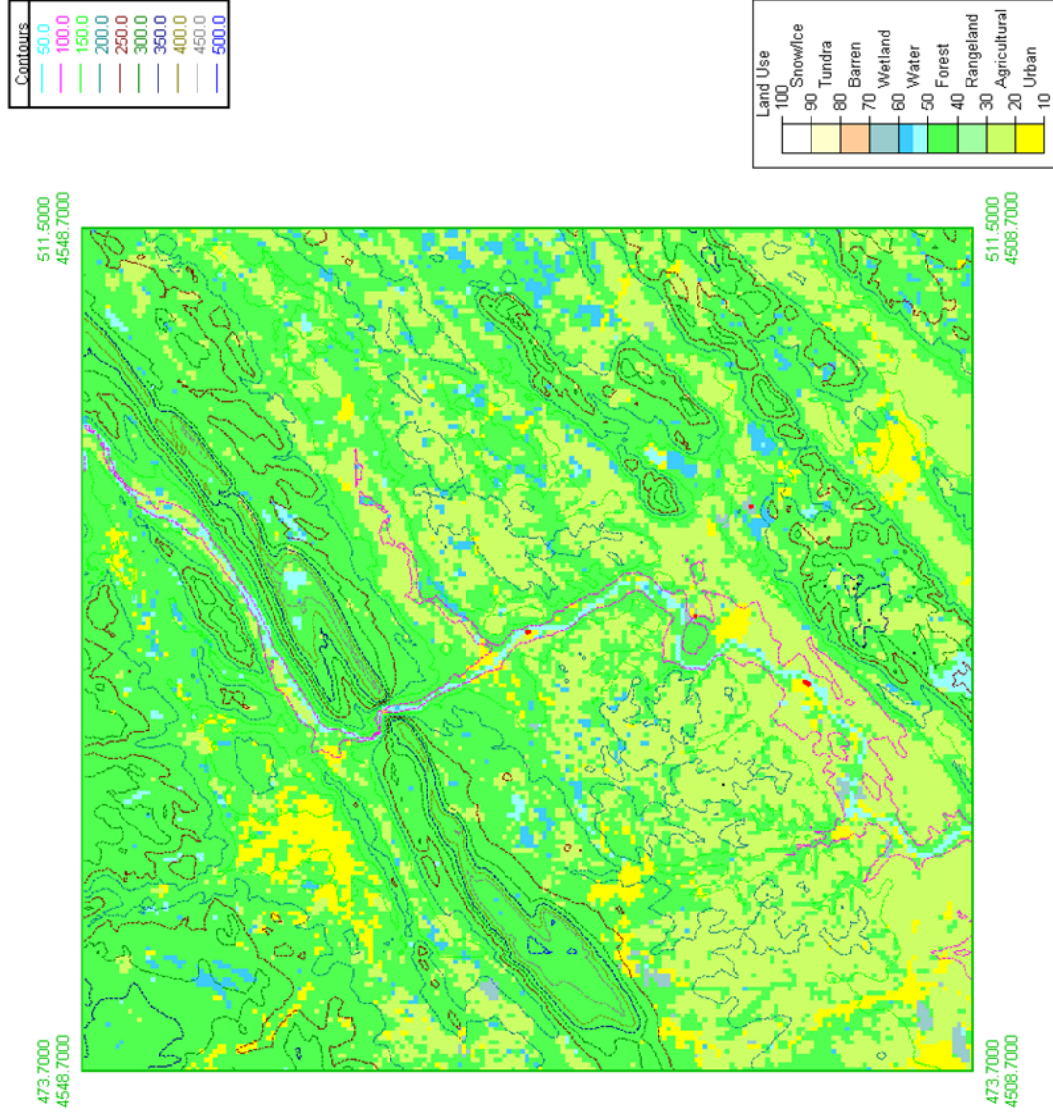


Figure 7. CALMET/CALPUFF Meteorological Modeling Domain with CALMET Processed Terrain and Land use Data

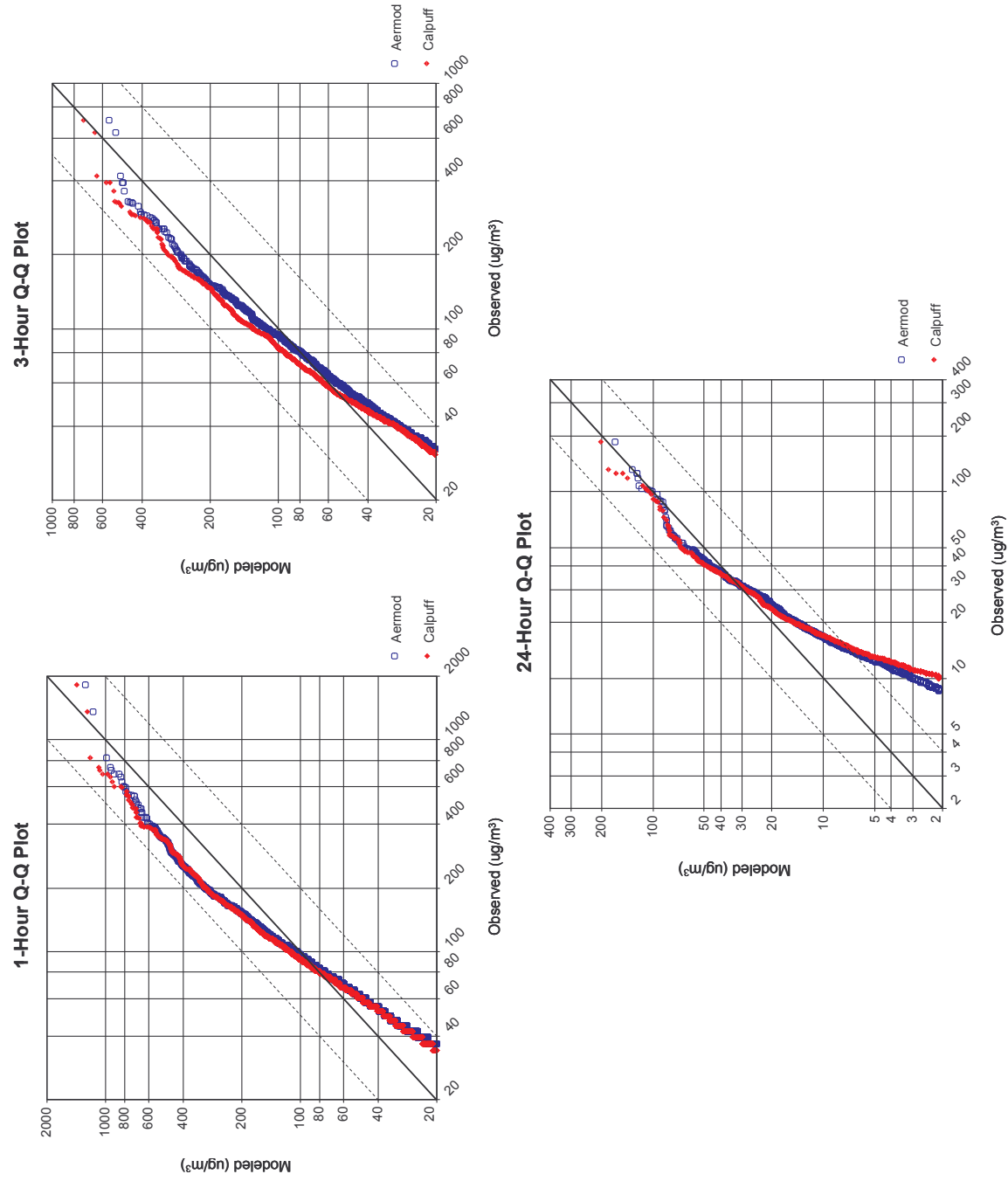


Figure 8. Q-Q Plots of CALPUFF and AERMOD Predicted Concentrations and Observed Concentrations

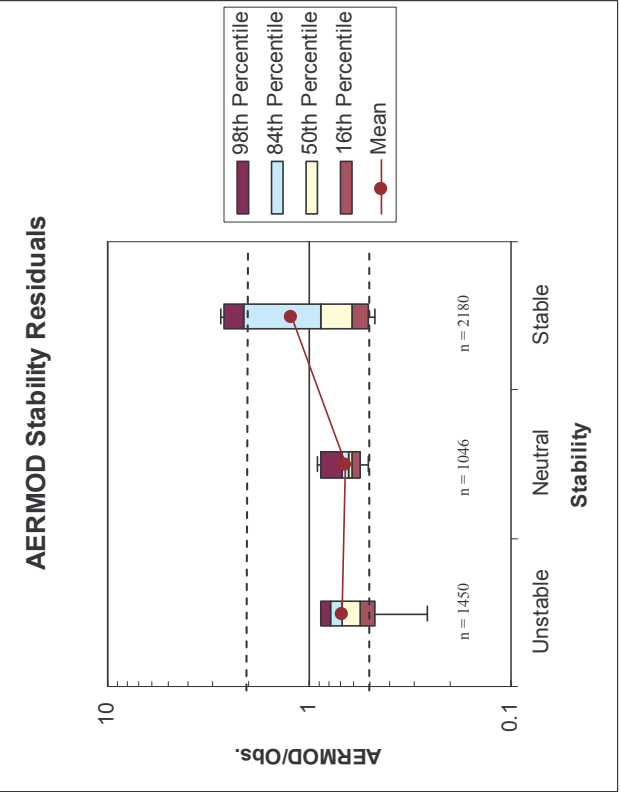
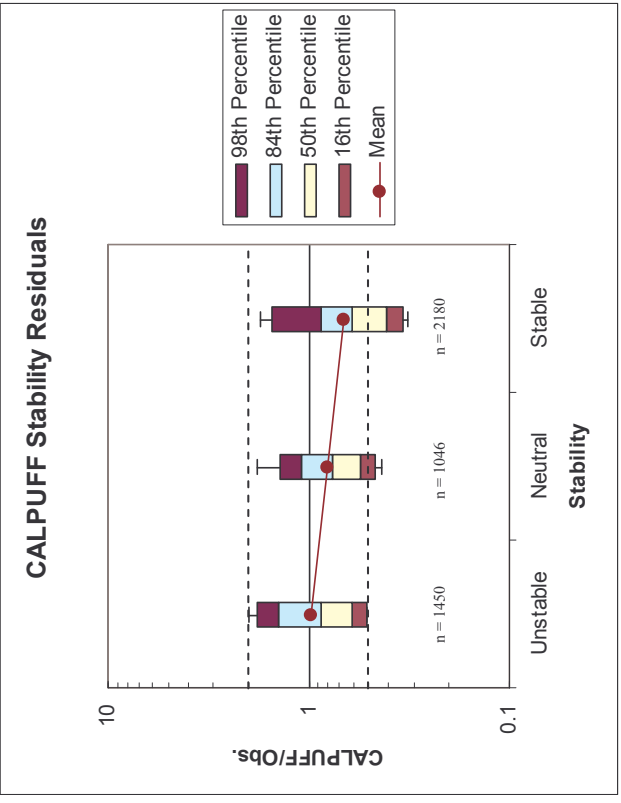
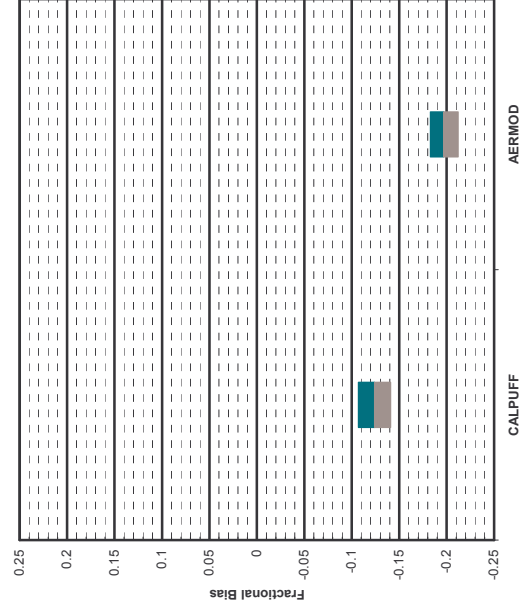


Figure 9. Residual Box Plots of 1-hr Model Residuals as a Function of Atmospheric Stability

Network 1-Hour Ranked Fractional Bias with 95% Confidence Limits



Network 1-Hour Peak Time Series Fractional Bias with 95% Confidence Limits

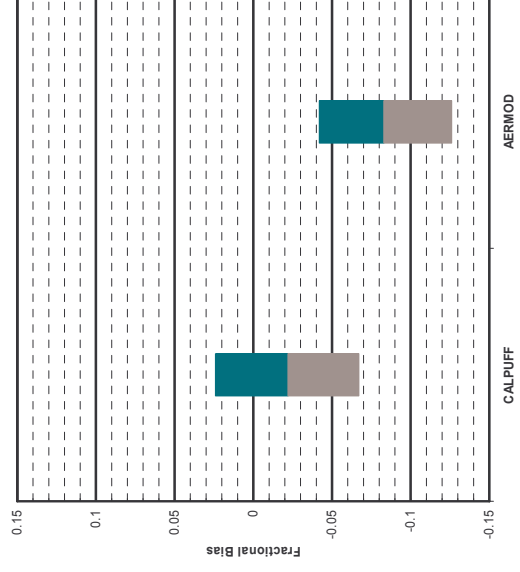


Figure 10. Fractional Bias Confidence Limits for the 1-hour Network Ranked and Time Series Data Pairings

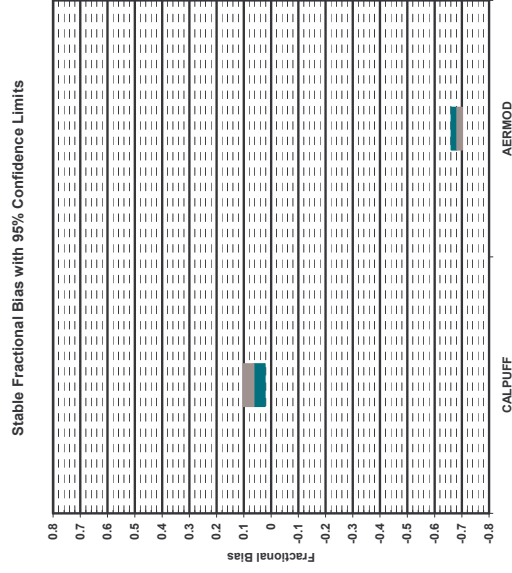
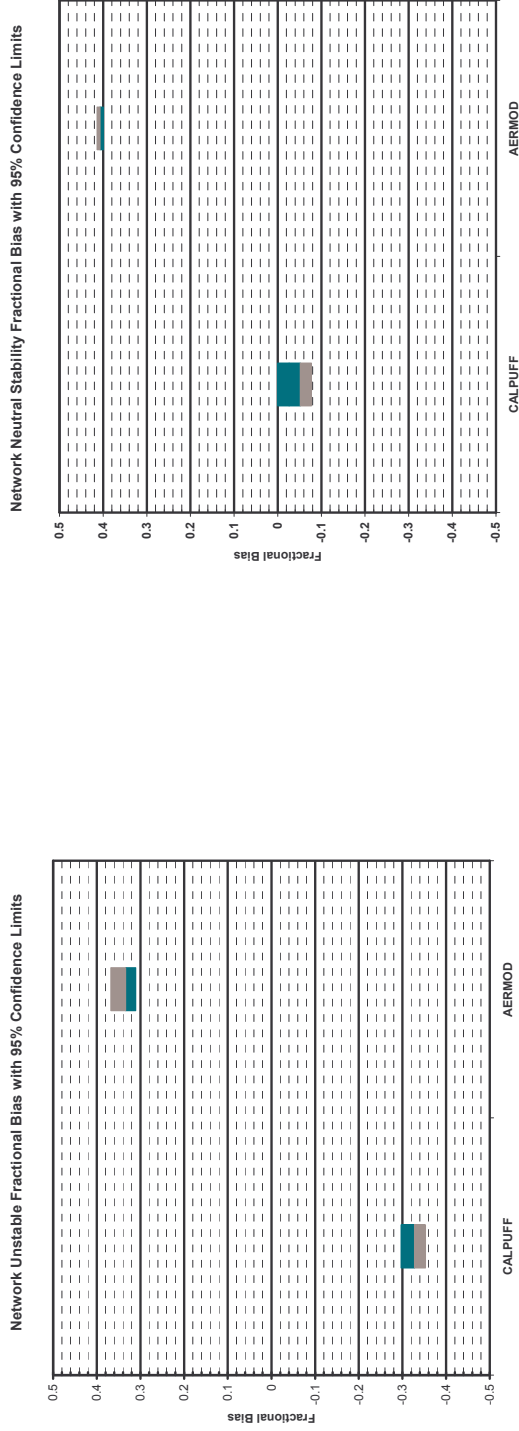


Figure 11. 1-hour Fractional Bias Confidence Limits as a Function of Atmospheric Stability



Photo 1. Martins Creek Power Plant with Scotts Mountain in Background



Photo 2. Portland Power Plant with New Jersey in the Background (Southeast Perspective)



Photo 3. Looking South with Portland Power Plant in the Foreground and Martins Creek in the Background



Photo 4. View of the Portland Power Plant through the Delaware Water Gap and Kittatinny Ridge (Southeast Perspective)

APPENDIX A

Example AERMOD Modeling File

```

*** AERMOD - VERSION 07026 ***      *** DEP Evaluation of AERMOD : Martin's Creek 1992-93      ***
*** AERMET-06341 and Prime ***      10/23/09
***                                     ***      10:58:58
**MODELOPTS:                                     ***      PAGE 1
CONC      DEFAULT ELEV

- - - - -      ***      MODEL SETUP OPTIONS SUMMARY      ***
- - - - -

**Model Is Setup For Calculation of Average Concentration Values.

-- DEPOSITION LOGIC --
**Model Uses NO DRY DEPLETION.  DDPLETE = F
**Model Uses NO WET DEPLETION.  WDPLETE = F
**NO GAS DRY DEPOSITION Data Provided.

**Model Uses RURAL Dispersion Only.

**Model Uses Regulatory DEFAULT Options:
1. Stack-tip Downwash.
2. Model Accounts for ELEVated Terrain Effects.
3. Use Calms Processing Routine.
4. Use Missing Data Processing Routine.
5. No Exponential Decay

**Model Assumes No FLAGPOLE Receptor Heights.

**Model Calculates 3 Short Term Average(s) of: 1-HR 3-HR 24-HR
and Calculates PERIOD Averages

**This Run Includes: 8 Source(s); 3 Source Group(s); and 8 Receptor(s)

**The Model Assumes A Pollutant Type of: SO2

**Model Set To Continue RUNNING After the Setup Testing.

**Output Options Selected:
Model Outputs Tables of PERIOD Averages by Receptor
Model Outputs Tables of Highest Short Term Values by Receptor (RECTABLE Keyword)
Model Outputs Tables of Overall Maximum Short Term Values (MAXTABLE Keyword)
Model Outputs External File(s) of High Values for Plotting (PLOTFILE Keyword)
Model Outputs External File(s) of Ranked Values (RANKFILE Keyword)

**NOTE: The Following Flags May Appear Following CONC Values: c for Calm Hours
m for Missing Hours
b for Both Calm and Missing Hours

**Misc. Inputs: Base Elev. for Pot. Temp. Profile (m MSL) = 73.20 ; Decay Coef. = 0.000 ; Rot. Angle = 0.0
Emission Units = GRAMS/SEC ; Emission Rate Unit Factor = 0.10000E+07
Output Units = MICROGRAMS/M**3

```

**Approximate Storage Requirements of Model = 1.3 MB of RAM.

**Input Runstream File: MartinsCreek_9293_coord_1992_SO2.DTA
**Output Print File: MartinsCreek_9293_coord_1992_SO2.LST
**Detailed Error/Message File: U:\AERMOD-CALPUFF_Eval_DEP\AERMOD\ncrat2.err

** AERMOD - VERSION 07026 *** ** DEP Evaluation of AERMOD : Martin's Creek 1992-93 *** 10/23/09
*** AERMET-06341 and Prime *** 10:58:58
**MODELOPTs: PAGE 2
CONC

DEFAULT ELEV

*** POINT SOURCE DATA ***

SOURCE ID	NUMBER PART. CATS.	EMISSION RATE (GRAMS/SEC)	X (METERS)	Y (METERS)	BASE ELEV. (METERS)	STACK HEIGHT (METERS)	STACK TEMP. (DEG.K)	STACK EXIT VEL. (M/SEC)	STACK DIAMETER (METERS)	BLDG EXISTS	URBAN SOURCE	CAP/ HOR	EMIS RATE SCALAR	VARY BY
MC12	0	0.10000E+01	491020.0	515910.0	73.2	182.90	422.00	28.30	5.30	YES	NO	NO	HOURLY	
MC3	0	0.10000E+01	491123.0	516030.0	71.7	182.90	422.00	33.50	6.90	YES	NO	NO	HOURLY	
MC4	0	0.10000E+01	491190.0	516068.0	69.8	182.90	422.00	33.50	6.90	YES	NO	NO	HOURLY	
ED1	0	0.10000E+01	493349.0	528506.0	89.6	121.90	403.10	43.30	2.84	NO	NO	NO	HOURLY	
ED2	0	0.10000E+01	493335.0	528554.0	89.6	121.90	405.90	36.30	3.60	NO	NO	NO	HOURLY	
HL2	0	0.10000E+01	494050.0	521040.0	103.6	59.40	419.00	16.90	2.70	NO	NO	NO	HOURLY	
WC1	0	0.10000E+01	498950.0	518500.0	173.7	76.20	389.00	16.30	1.87	NO	NO	NO	HOURLY	
WC2	0	0.10000E+01	498950.0	518500.0	173.7	76.20	389.00	16.30	1.87	NO	NO	NO	HOURLY	

** AERMOD - VERSION 07026 *** ** DEP Evaluation of AERMOD : Martin's Creek 1992-93 *** 10/23/09
*** AERMET-06341 and Prime *** 10:58:58
**MODELOPTs: PAGE 3
CONC

DEFAULT ELEV

*** SOURCE IDS DEFINING SOURCE GROUPS ***

SOURCE IDS

GROUP ID

ALL MC12 , MC3 , MC4 , ED1 , ED2 , HL2 , WC1 , WC2 ,

NJDEP

Division of Air Quality

Bureau of Technical Services

Page 54

2/25/2010

MC MC12 , MC3 , MC4 ,

PORTLAND ED1 , ED2 ,

*** AERMOD - VERSION 07026 *** ** DEP Evaluation of AERMOD : Martin's Creek 1992-93
*** AERMET-06341 and Prime

**MODELOPTs:

CONC DEFAULT ELEV

10/23/09
10:58:58
PAGE 4

*** DIRECTION SPECIFIC BUILDING DIMENSIONS ***

SOURCE ID: MC12

IFV	BH	BW	BL	XADJ	YADJ	IFV	BH	BW	BL	XADJ	YADJ
1	0.0,	0.0,	0.0,	0.0,	0.0,	2	0.0,	0.0,	0.0,	0.0,	0.0,
3	0.0,	0.0,	0.0,	0.0,	0.0,	4	0.0,	0.0,	0.0,	0.0,	0.0,
5	0.0,	0.0,	0.0,	0.0,	0.0,	6	0.0,	0.0,	0.0,	0.0,	0.0,
7	0.0,	0.0,	0.0,	0.0,	0.0,	8	0.0,	0.0,	0.0,	0.0,	0.0,
9	0.0,	0.0,	0.0,	0.0,	0.0,	10	0.0,	0.0,	0.0,	0.0,	0.0,
11	0.0,	0.0,	0.0,	0.0,	0.0,	12	0.0,	0.0,	0.0,	0.0,	0.0,
13	0.0,	0.0,	0.0,	0.0,	0.0,	14	0.0,	0.0,	0.0,	0.0,	0.0,
15	0.0,	0.0,	0.0,	0.0,	0.0,	16	0.0,	0.0,	0.0,	0.0,	0.0,
17	90.0,	200.1,	137.9,	-421.0,	136.7,	18	90.0,	203.0,	161.0,	-451.0,	73.5,
19	90.0,	199.7,	179.2,	-467.2,	8.1,	20	90.0,	190.4,	192.0,	-469.3,	-57.7,
21	90.0,	175.3,	198.9,	-457.1,	-121.6,	22	0.0,	0.0,	0.0,	0.0,	0.0,
23	0.0,	0.0,	0.0,	0.0,	0.0,	24	0.0,	0.0,	0.0,	0.0,	0.0,
25	0.0,	0.0,	0.0,	0.0,	0.0,	26	0.0,	0.0,	0.0,	0.0,	0.0,
27	0.0,	0.0,	0.0,	0.0,	0.0,	28	0.0,	0.0,	0.0,	0.0,	0.0,
29	0.0,	0.0,	0.0,	0.0,	0.0,	30	0.0,	0.0,	0.0,	0.0,	0.0,
31	0.0,	0.0,	0.0,	0.0,	0.0,	32	0.0,	0.0,	0.0,	0.0,	0.0,
33	0.0,	0.0,	0.0,	0.0,	0.0,	34	0.0,	0.0,	0.0,	0.0,	0.0,
35	0.0,	0.0,	0.0,	0.0,	0.0,	36	0.0,	0.0,	0.0,	0.0,	0.0,

SOURCE ID: MC3

IFV	BH	BW	BL	XADJ	YADJ	IFV	BH	BW	BL	XADJ	YADJ
1	90.0,	199.7,	179.2,	152.0,	72.6,	2	90.0,	190.4,	192.0,	129.3,	113.4,
3	0.0,	0.0,	0.0,	0.0,	0.0,	4	0.0,	0.0,	0.0,	0.0,	0.0,
5	0.0,	0.0,	0.0,	0.0,	0.0,	6	0.0,	0.0,	0.0,	0.0,	0.0,
7	0.0,	0.0,	0.0,	0.0,	0.0,	8	0.0,	0.0,	0.0,	0.0,	0.0,
9	0.0,	0.0,	0.0,	0.0,	0.0,	10	0.0,	0.0,	0.0,	0.0,	0.0,
11	0.0,	0.0,	0.0,	0.0,	0.0,	12	0.0,	0.0,	0.0,	0.0,	0.0,
13	0.0,	0.0,	0.0,	0.0,	0.0,	14	90.0,	194.6,	129.7,	-275.7,	138.4,
15	90.0,	183.6,	100.6,	-282.0,	99.7,	16	90.0,	191.1,	110.6,	-300.8,	58.0,
17	90.0,	200.1,	137.9,	-320.8,	14.4,	18	90.0,	203.0,	161.0,	-331.0,	-29.5,
19	90.0,	199.7,	179.2,	-331.2,	-72.6,	20	90.0,	190.4,	192.0,	-321.3,	-113.4,
21	0.0,	0.0,	0.0,	0.0,	0.0,	22	0.0,	0.0,	0.0,	0.0,	0.0,

NJDEP

Division of Air Quality
Bureau of Technical Services

Page 55

2/25/2010


```

*** AERMOD - VERSION 07026 ***      *** DEP Evaluation of AERMOD : Martin's Creek 1992-93
***                                     *** AERMET-06341 and Prime
***                                     ***
*** MODELOPTS:
CONC                                DEFAULT ELEV
***                                     ***
***                                     ***
10/23/09                            10:58:58
PAGE 6

```

*** METEOROLOGICAL DAYS SELECTED FOR PROCESSING ***
(1=YES; 0=NO)

[illegible]

METEOROLOGICAL DATA PROCESSED BETWEEN START DATE: 0 0 0 0
AND END DATE: 9999 99 99 24

NOTE: METEOROLOGICAL DATA ACTUALLY PROCESSED WILL ALSO DEPEND ON WHAT IS INCLUDED IN THE DATA FILE.

*** UPPER BOUND OF FIRST THROUGH FIFTH WIND SPEED CATEGORIES ***
(METERS/SEC)

1.54, 3.09, 5.14, 8.23, 10.80,

```

*** AERMOD - VERSION 07026 ***      *** DEP Evaluation of AERMOD : Martin's Creek 1992-93 *** 10/23/09
***                                     *** AERMET-06341 and Prime ***                        10:58:58
***                                     ***                                     ***                        PAGE 7
**MODELOPTs:
CONC                                     DEFAULT ELEV

```

*** UP TO THE FIRST 24 HOURS OF METEOROLOGICAL DATA ***

```

Surface file:  MC_sequoia.SFC
Profile file:  MC_sequoia.PFL
Surface format:  FREE
Profile format:  FREE
Surface station no.:  14737
Name:  ALLENTOWN,PA
Year:  1992

Upper air station no.:  14735
Name:  ALBANY,NY
Year:  1992

```

First 24 hours of scalar data																						
YR	MO	DY	JDY	HR	H0	U*	W*	DT/DZ	ZICNV	ZIMCH	M-O	LEN	Z0	BOWEN	ALBEDO	REF	WS	WD	HT	REF	TA	HT
92	05	01	122	01	-0.1	0.011	-9.000	-9.000	-999.	11.		1.4	0.05	1.07	1.00	0.30	300	300	10.0	283.1	10.0	

APPENDIX B

CALMET and CALPUFF Inputs

Table B.1 Important CALMET Control File Variables			
Variable	Description	Default	Value
NUSTA	Number of upper air stations	NA	4
IBYR	Starting Date: Year	NA	1992
IBMO	Starting Date: Month	NA	5
IBDY	Starting Date: Day	NA	1
IBHR	Starting Date: Hour	NA	1
IBTZ	Base Time Zone	NA	5
IRLG	Length of run (hours)	NA	9239
IRTYPE	Run type 0= compute wind fields only 1= compute wind fields and micrometeorological variables	1	1
LCALGRID	Compute special data fields required for CALGRID	T	F
ITEST	Flag to stop run after setup 1= stop 2= continue	2	2
MREG	Test options to see if they conform to regulatory values	na	0 No
PMAP	Map projection	na	UTM
NX	No. of X grid cells	Na	189
NY	No. of Y grid cells	Na	200
DGRIDKM	Grid spacing (km)	Na	0.200
XORIGKM	X coordinate (km)	Na	473.700
YORIGKM	Y coordinate (km)	Na	4508.700
NZ	No. Vertical layers	Na	12
ZFACE	Cell heights in grid	Na	0, 20, 40, 80, 135, 195, 255, 315, 405, 1000, 1500, 2200, 3000
NOOBS	No. observation mode (0 = surface, overwater and upper air)	0	0
NSSTA	No. of surface meteorological stations	Na	5
NPSTA	No. of precipitation stations (-1 to use MM5)	na	0
ICLOUD	Gridded cloud fields (0 = not used)	0	0
IWFCOD	Model selection variable	1	1
IFRADJ	Compute Froude number adjustment? (0 = no, 1 = yes)	1	1
IKINE	Compute kinematic effects? (0 = no, 1 = yes)	0	0

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Division of Air Quality

Bureau of Technical Services

Table B.1 Important CALMET Control File Variables			
Variable	Description	Default	Value
IOBR	Use O'Brien procedure? (0 = no, 1 = yes)	0	0
ISLOPE	Compute slope flow effects? (0 = no, 1 = yes)	1	1
IEXTRP	Extrapolate surface wind observations to upper levels?	-4	-4
ICALM	Extrapolate surface winds even if calm? (0 = no, 1 = yes)	0	1
BIAS	Layer dependent biases modifying the weights of surface and upper air stations	NA	-1 first layer, 0 next two layers,+1 other 9
RMIN2	Minimum distance from nearest upper air station to surface station for which extrapolation of surface winds at surface station will be allowed (set to -1 for IEXTRP where all surface stations should be extrapolated)	4	-1
IPROG	Use gridded prognostic wind field model output fields as input to the diagnostic wind field model (0 = no)	0	0
ISTEPPG	Time step (hours) of the prognostic model input data	1	1
LVARY	Use varying radius of influence	F	F
RMAX1	Maximum radius of influence over land (km)	Na	2
RMAX2	Maximum radius of influence over land aloft (km)	Na	2
RMAX3	Maximum radius of influence over water (km)	Na	2
RMIN	Minimum radius of influence used in the wind field interpolation (km)	0.1	0.1
TERRAD	Radius of influence of terrain features (km)	NA	2.7
R1	Relative weighting of the first guess field and observations in the surface layer. (km)	NA	1
R2	Relative weighting of the first guess field and observations in the layers aloft. (km)	NA	1
ISURFT	No of surface stations.	NA	5

Table B.2 Important CALPUFF Control File Variables			
Variable	Description	Default	Value
IBYR	Starting Date: Year	NA	1992
IBMO	Starting Date: Month	NA	5
IBDY	Starting Date: Day	NA	1
IBHR	Starting Date: Hour	NA	1
IBTZ	Base Time Zone	NA	5
IRLG	Length of run (hours)	NA	9215
NSPEC	Number of chemical species	5	1
NSE	Number of chemical species emitted	3	1
METFM	Meteorological data format 1 = CALMET binary	1	1
MGAUSS	Vertical distribution used in the near field 1 = Gaussian	1	1
MCTADJ	Terrain adjustment method 3 = partial plume path adj.	3	3
MSLUG	Near-field puffs modeled as elongated slugs? 1 = yes	0	0
MTRANS	Transitional plume rise modeled? 1 = yes	1	1
MTIP	Stack tip downwash modeled? 1 = yes	1	1
MBDW	Method used to simulate building downwash 1 = ISC	1	1
MSHEAR	Vertical wind shear modeled above stack top? 0 = no	0	0
MSPLIT	Puff splitting allowed? 0 = no	0	0
MCHEM	Chemical mechanism flag 1 = MESOPUFF II scheme	1	0
MAQCHEM	Aqueous phase transformation 0 = not modeled	0	0
MDISP	Method used to compute dispersion coefficients 2 = dispersion coefficients from internally calculated sigma v, sigma w. 3 = PG and MP dispersion coefficients	3	2
MCTURB	Method used to compute turbulence sigma-v & sigma-w using micrometeorological variables 1 = Calpuff 2 = Aermod	1	2
MPARTL	Partial plume penetration of elevated inversion? 1 = yes	1	1
MPDF	PDF dispersion under convective conditions? 1 = yes	0	1
CSPEC	Chemical species modeled	na	SO ₂
CSPEC	Chemical species emitted	na	SO ₂
MOZ	Ozone data input option 1 = hourly ozone conc	1	0

APPENDIX C

Determination of Robust High Concentrations (RHC)

The robust high concentration (RHC) is designed to represent a smoothed estimate of the highest concentration based on an exponential fit to the upper end of the concentration distribution. The RHC attempts to represent a stable estimate of the highest concentration, one that mitigates the unwanted influence of unusual events. As stated in the AERMOD validation study (Perry, et. al., 2005), “for regulatory applications, a good model would produce a concentration distribution parallel to the slope of the measured distribution and produce high-end concentrations (RHCs) that are similar to that of the observations.”

The guidance given on the selection of N is that the value needs to be large enough to adequately define the upper end of the distribution of concentrations. Because the upper end distribution of monitored concentrations will vary, the number of samples needed to define the upper end of the concentration distribution (N) for a given set of data may vary. Therefore, each upper end distribution of concentrations must be evaluated on an individual basis and value of N selected that best defines the slope. The apriori selection of N as 26 without examination of the data is arbitrary (Cox and Tikvart, 1990; EPA, 1992) and can result in the use of an inaccurate RHC value.

The highest 51 network 3-hour monitored concentrations are graphed in Figure C.1. Examination of the figure indicates that beginning with the 8th highest concentration, the 3-hour monitored values increase rapidly defining the upper end distribution. The calculated 3-hour RHC based on the eight highest concentrations is slightly below the actual monitored 3-hour maximum (659 $\mu\text{g}/\text{m}^3$ vs. 710 $\mu\text{g}/\text{m}^3$).

The highest 51 network 24-hour monitored concentrations are graphed in Figure C.2. In this case, the 24-hour monitored values begin increasing at a much higher rate near the 26th highest value. Therefore, these concentrations represent the upper end distribution and are used to define the 24-hour RHC. The calculated 24-hour RHC based on the 26 highest concentrations is very near the actual monitored 24-hour maximum (185.3 $\mu\text{g}/\text{m}^3$ vs. 187 $\mu\text{g}/\text{m}^3$).

The highest 51 3-hour concentrations measured at AMS#12, the single monitor with the highest overall 3-hour concentrations, are graphed in Figure C.3. Examination of the figure indicates that beginning with the 11th highest concentration, the 3-hour monitored values increase rapidly defining the upper end distribution. The calculated 3-hour RHC based on the 11 highest concentrations is below the actual monitored 3-hour maximum (506.2 $\mu\text{g}/\text{m}^3$ vs 629.7 $\mu\text{g}/\text{m}^3$).

The highest 51 24-hour concentrations measured at AMS#8, the single monitor with the highest overall 24-hour concentrations, are graphed in Figure C.4. In this case, the 24-hour monitored values begin increasing at a much higher rate near the 16th highest value. Therefore, these concentrations represent the upper end distribution and should be used to define the 24-hour

RHC. The calculated 24-hour RHC based on the 16 highest concentrations at AMS#8 is slightly above the actual monitored 24-hour maximum (185.3 ug/m³ vs. 194.6 ug/m³).

For the scientific component, two categories of monitors were evaluated for three different atmospheric stabilities. One category of monitors were those located in complex terrain at or above plume height (AMS-5, -7, -9, -10, -11, -12, and -13). The other category represents a monitor (AMS-8) located at approximately stack top. The three atmospheric stabilities classes are unstable, neutral, and stable.

The highest 51 1-hour monitored concentrations measured at AMS-5, -7, -9, -10, -11, -12, and -13 (complex terrain monitors) for the three atmospheric stabilities are graphed in Figure C.5. The 1-hour monitored values begin increasing at a higher rate at different points in the concentration distribution for each stability. Therefore, RHCs of 8 (unstable), 23 (neutral), and 19 (stable) were selected to represent the upper end distribution of monitored concentrations. Figure C.5 shows the calculated 1-hour RHC for all stabilities are below the actual monitored 1-hour maximum concentrations.

The highest 51 1-hour monitored concentrations measured at AMS-8 for the three stabilities are graphed in Figure C.6. The 1-hour monitored values begin increasing at a higher rate near the 26th highest value for the unstable case, at the 6th highest value for the neutral cases, and near the 11th high value for the stable case. Therefore, these concentrations and above represent the upper end distribution and are used to define the 1-hour RHC. As can be seen in Figure C.6, the calculated 1-hour RHC concentrations are very near the maximum monitored concentration for unstable and stable conditions, and below the actual monitored 1-hour maximum for neutral stability.

References

Cox, W., and J. Tikvart, 1990. A statistical procedure for determining the best performing air quality simulation model. *Atmos. Environ.* **24A**, 2387-2395.

United States Environmental Protection Agency, 1992. Protocol for Determining the Best Performing Model. EPA-454/R-92-025.

Perry, S. G., A. J. Cimorelli, R. J. Paine, R. W. Brode, J. C. Weil, A Venkatram, R. B. Wilson, R. F. Lee, and W.D. Peters. AERMOD: A dispersion model for industrial source applications. Part II: Model performance against 17 field study databases. *J Appl Meteor.*, **44**, 694-708.

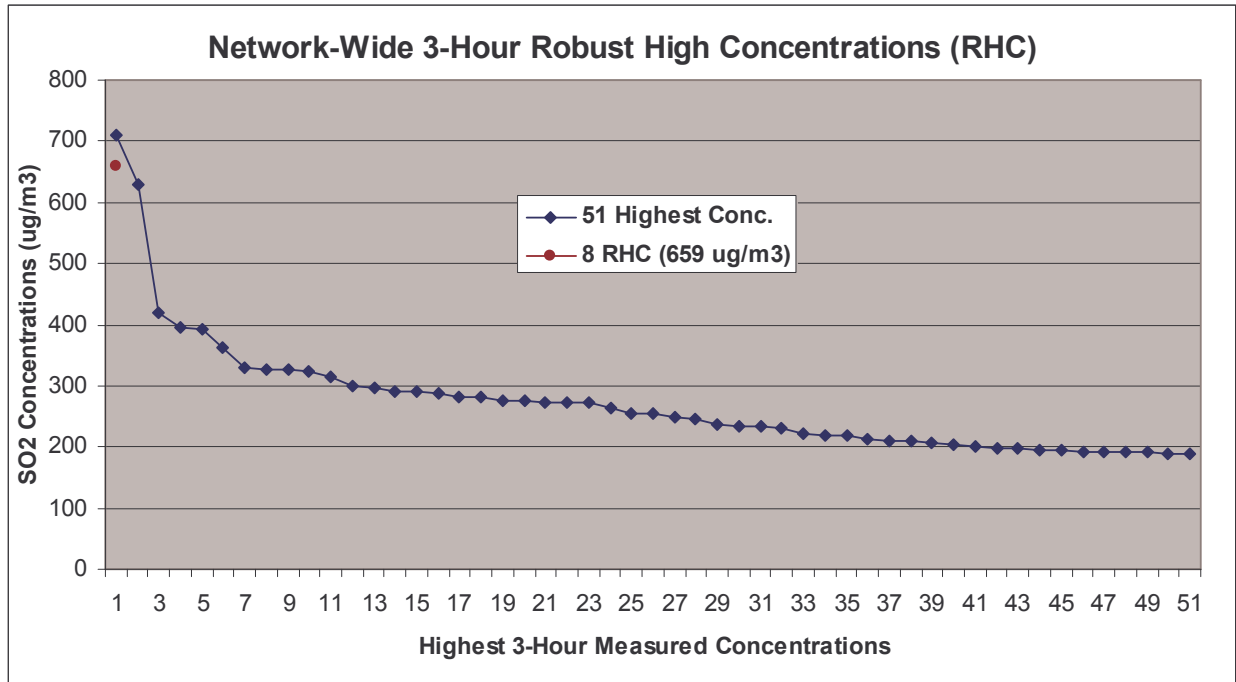


Figure C.1.

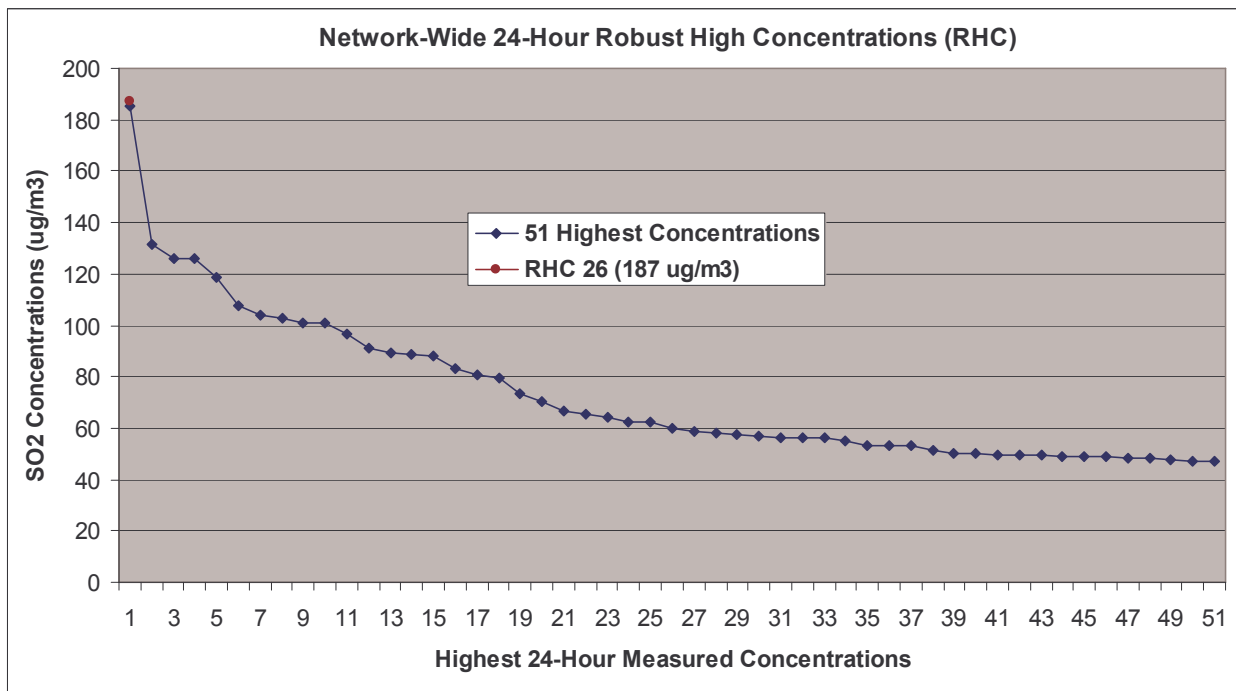


Figure C.2.

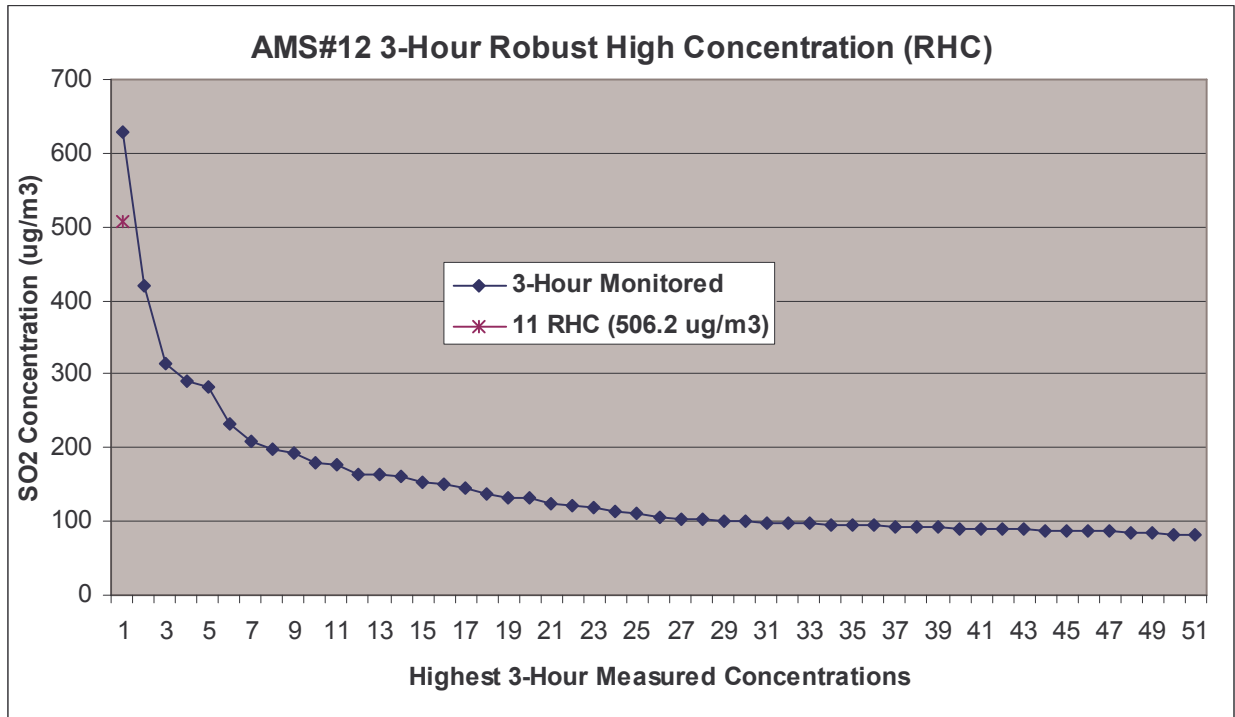


Figure C.3

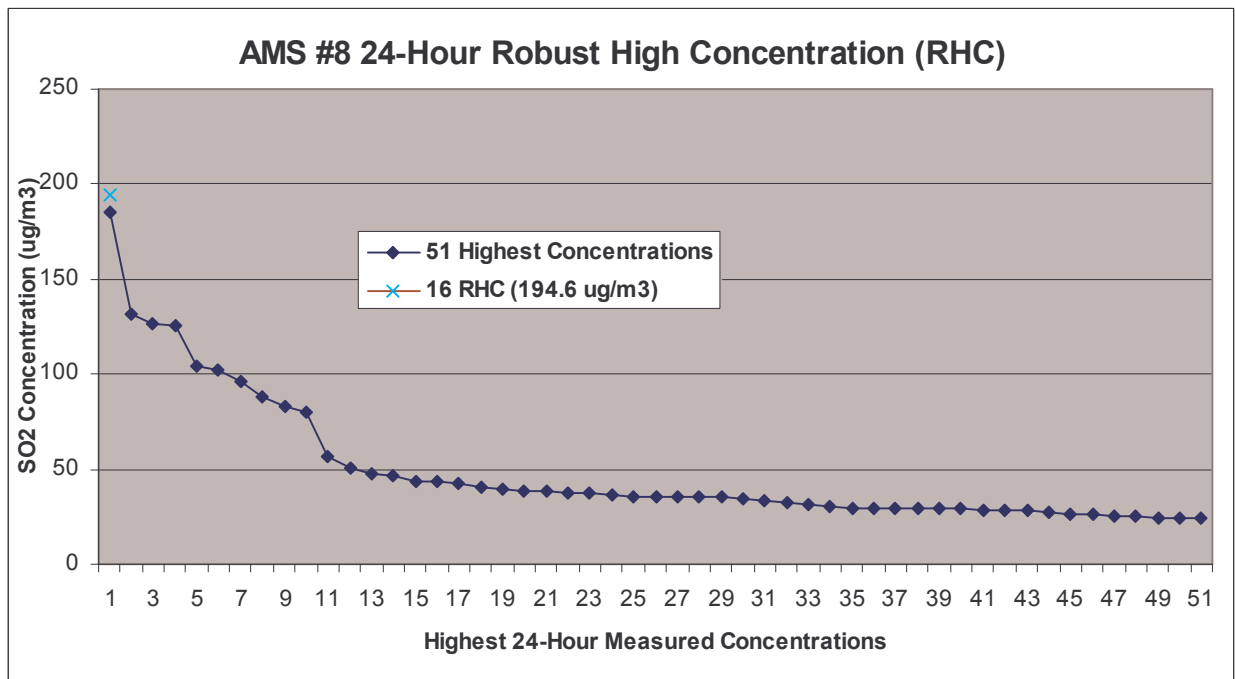


Figure C.4

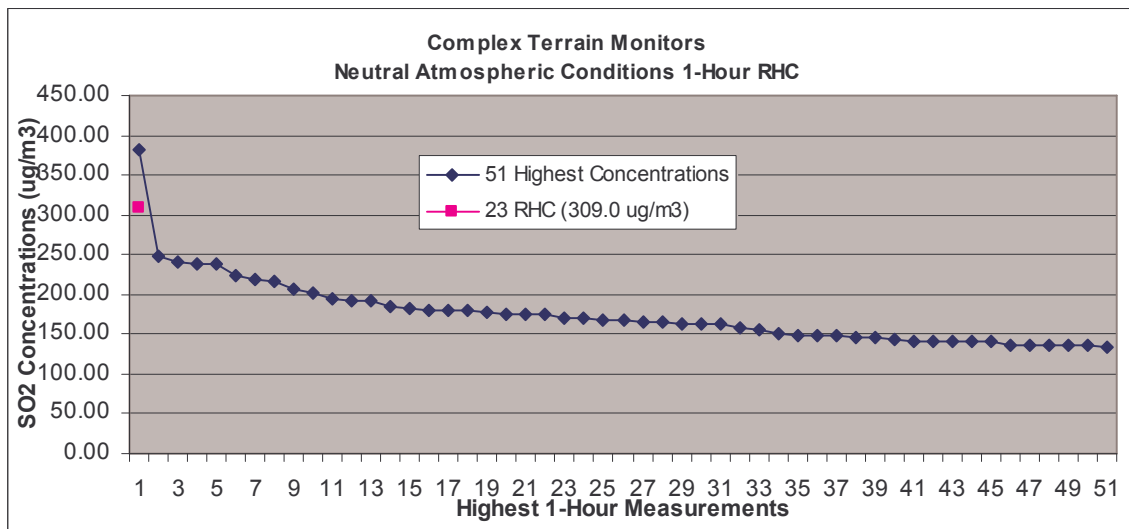
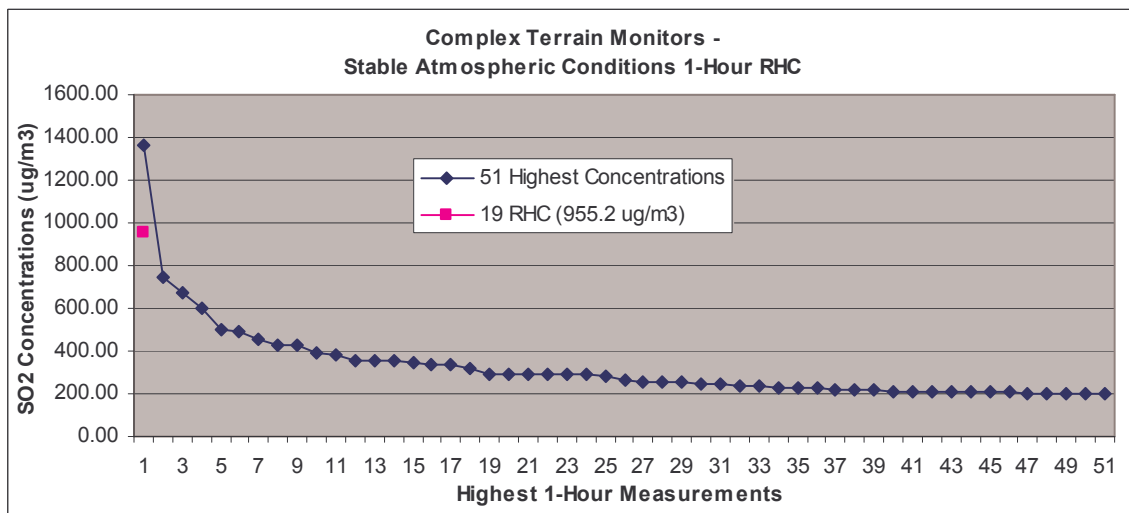
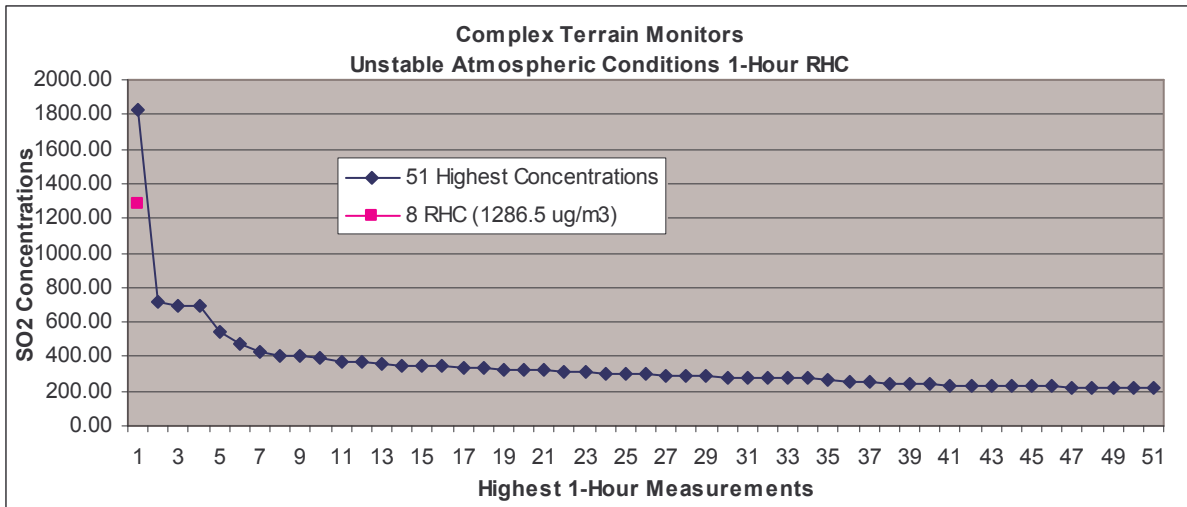


Figure C.5

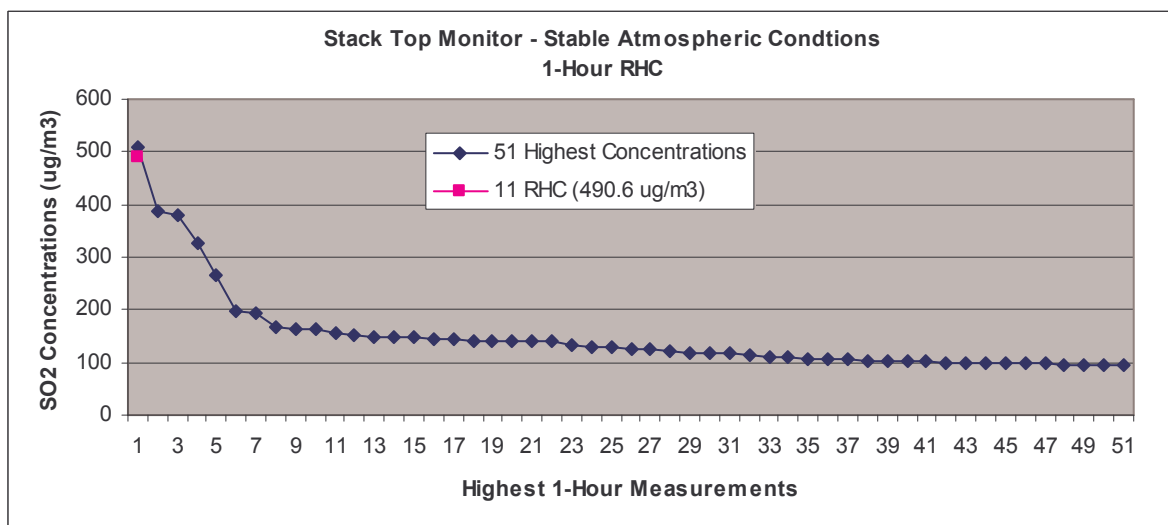
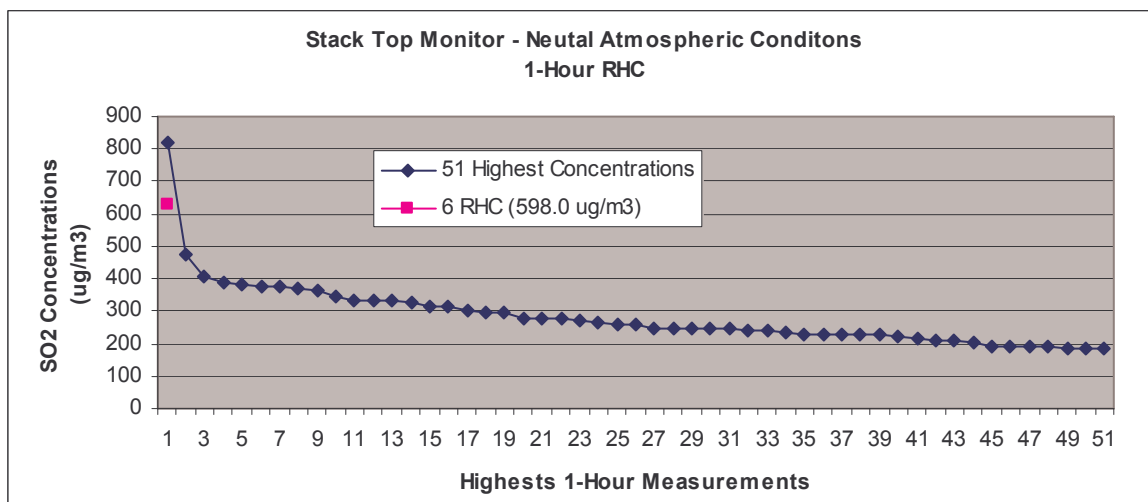
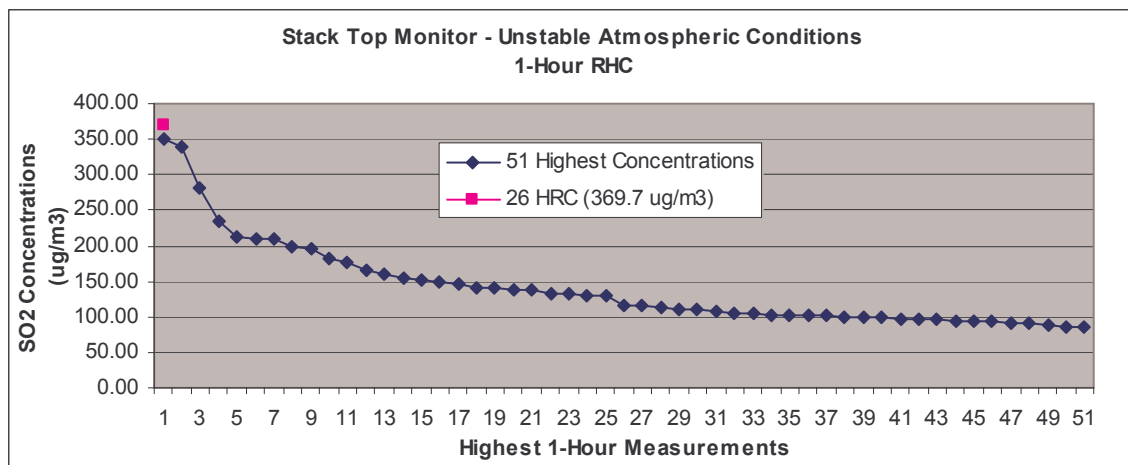


Figure C.6